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MODELING OF RIVER HYDRODYNAMICS AND ACTIVE CAP EFFECTIVENESS IN
THE ANACOSTIA RIVER

A Thesis

Submitted to the Graduate Faculty of the
Louisiana State University and
Agricultural and Mechanical College
In partial fulfillment of the
Requirements for the degree of
Master of Science in Civil Engineering

In

The Department of Civil and Environmental Engineering

by
Keegan L. Roberts
BS, Louisiana State University, 2001
December 2004

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Table of Contents

Acknowledgements.....	ii
Abstract.....	viii
Chapter 1: Introduction.....	1
1.1 Anacostia River Demonstration Site Description.....	3
1.2 HSRC Anacostia Remediation Effort.....	6
1.3 Literature Review.....	7
1.3.1 Review of Previous Anacostia River Hydrodynamic Studies.....	7
1.3.2 Review of Previous Anacostia River Sediment Transport Studies.....	9
1.3.3 Review of Previous Anacostia River Chemical Fate and Transport Studies.....	9
1.3.4 Review of Alternative Predictive Hydrologic Modeling Software Packages.....	9
1.3.5 Review of Alternative Predictive Sediment Transport Modeling Software Packages.....	10
1.3.6 Review of Alternative Predictive Chemical Transport Modeling Software Packages.....	11
1.3.7 MARS Model Hierarchy.....	11
1.4 Research Objectives.....	11
Chapter 2: Hydrodynamic Modeling of the Anacostia River.....	14
2.1 Description of Grid Generation for MARS Model.....	14
2.2 Description of MARS Hydrodynamic Model Variables and Inputs.....	15
2.2.1 Length of Simulation.....	15
2.2.2 Print Interval.....	16
2.2.3 Dimensionless Drag Coefficient.....	17
2.2.4 Horizontal Dispersion Parameter.....	17
2.2.5 Tidal/River Variable.....	18
2.2.6 a, b, and c in the Depth-Flow Function.....	18
2.2.7 12-hour and 24-hour Tidal Phase.....	19
2.2.8 12-hour and 24-hour Tidal Amplitudes.....	20
2.2.9 Depth Shift.....	20
2.2.10 Water Column Depth.....	20
2.2.11 Flow Rate.....	21
2.3 Development of MARS Hydrodynamic Model Variables and Inputs to Simulate Anacostia River Flow Events.....	22
2.3.1 Length of Simulation.....	22
2.3.2 Print Interval.....	23
2.3.3 Dimensionless Drag Coefficient.....	23
2.3.4 Horizontal Dispersion Parameter.....	23
2.3.5 Tidal/River Variable.....	23
2.3.6 a, b, and c in the Depth-Flow Function.....	24
2.3.7 12-hour and 24-hour Tidal Phase.....	26
2.3.8 12-hour and 24-hour Tidal Amplitudes.....	27
2.3.9 Depth Shift.....	27
2.3.10 Water Column Depth.....	27
2.3.11 Flow Rate.....	27

2.4 MARS Hydrodynamic Model Results	27
2.4.1 Hydrodynamic Model Results	28
2.5 Conclusions and Recommendations for Future Improvements	32
2.5.1 Conclusions	32
2.5.2 Recommendations for Future Improvements	32
Chapter 3: Sediment Transport Modeling of the Anacostia River	34
3.1 Description of MARS Hydrodynamic Model Variables and Inputs	35
3.1.1 Print Interval	36
3.1.2 Dry Density	36
3.1.3 Bottom Friction Coefficient	36
3.1.4 Initial Concentration	39
3.1.5 Boundary Concentration	39
3.1.6 α and β in Settling Equation	39
3.1.7 Critical Shear Stress for Erosion	41
3.1.8 a_o , n , and m in Sediment Erosion Equation	41
3.1.9 Upstream Concentration	42
3.1.10 Critical Shear Stress, Layers 1 through 7	42
3.1.11 Time Step	42
3.1.12 Wind Speed	42
3.1.13 Wind Direction	43
3.2 Development of MARS Sediment Transport Model Variables and Inputs to Simulate Anacostia River Sediment Transport Phenomena	43
3.2.1 Print Interval	43
3.2.2 Dry Density	43
3.2.3 Bottom Friction Coefficient	44
3.2.4 Initial Concentration	44
3.2.5 Boundary Concentration	45
3.2.6 α and β in Settling Equation	45
3.2.7 Critical Shear Stress	45
3.2.8 a_o , n , and m in Sediment Erosion Equation	45
3.2.9 Upstream Concentration	46
3.2.10 Critical Shear Stress, Layers 1 through 7	46
3.2.11 Time Step	47
3.2.12 Wind Speed	47
3.2.13 Wind Direction	47
3.3 MARS Sediment Transport Model Results	48
3.3.1 Sediment Transport Model Results	48
3.4 Conclusions and Recommendations for Future Improvements	53
3.4.1 Conclusions	53
3.4.2 Recommendations for Future Improvements	53
Chapter 4: Chemical Fate and Transport Modeling in Anacostia River Sediments	55
4.1 Description of MARS Chemical Fate and Transport Model Variables and Inputs	55
4.1.1 Dissolved and DOC Biodegradation Rate Constant at 20°C	56
4.1.2 Dissolved K_{bio} Temperature Correction	56

4.1.3 Sediment Dissolved and DOC Bacteria Density	57
4.1.4 Sediment Solids Bacteria Density.....	57
4.1.5 Solids Biodegradation Rate Constant at 20°C	57
4.1.6 Solids K_{bio} Temperature Correction.....	58
4.1.7 Water Column Dissolved & Dissolved Organic Carbon Bacteria Density	58
4.1.8 Water Column Solids Bacteria Density	58
4.1.9 Downstream Boundary Concentration.....	58
4.1.10 Upstream Boundary Concentration.....	59
4.1.11 Water Column Initial Concentration.....	59
4.1.12 Sediment DOC Koc-Solids Koc Ratio.....	59
4.1.13 Sediment Bed DOC Concentration.....	59
4.1.14 Water Column DOC Concentration.....	60
4.1.15 Water Column DOC Koc-Solids Koc Ration	60
4.1.16 Chemical Name.....	60
4.1.17 Print Interval	60
4.1.18 Sediment Bed Temperature.....	61
4.1.19 Water Column Temperature	61
4.1.20 Acid Hydrolysis Rate Constant at 20°C	61
4.1.21 Alkaline Hydrolysis Rate Constant at 20°C	62
4.1.22 Hydrolysis Rate Constant Temperature Correction.....	62
4.1.23 Neutral Hydrolysis Rate Constant at 20°C	63
4.1.24 Sediment Bed pH	63
4.1.25 Water Column pH.....	63
4.1.26 Sediment Layer Depth	63
4.1.27 Solids Density	63
4.1.28 Kow-Koc Intercept and Slope.....	64
4.1.29 log Kow.....	64
4.1.30 Sediment Bed Fraction Organic Carbon.....	64
4.1.31 Solids Dependent Partition Parameter	65
4.1.32 Water Column Fraction Organic Carbon.....	65
4.1.33 Chemical Molecular Weight.....	65
4.1.34 Henry's Law Constant	66
4.1.35 Volatilization Option	66
4.1.36 Bed Boundary Condition Scale Factor	67
4.1.37 Bed Boundary Condition Time Series Number	67
4.1.38 Groundwater Flow Scale Factor	67
4.1.39 Groundwater Flow Time Series Number.....	68
4.1.40 Initial Concentrations in Sediment Layers.....	68
4.1.41 Sediment Layer Diffusion Coefficients	68
4.1.42 Water Column-Sediment Interface Diffusion Coefficient.....	69
4.1.43 Sediment Bed Solids Concentration	69
4.1.44 Bed Boundary Condition Time Series Numbers 1-10	70
4.1.45 Groundwater Flow Time Series Numbers 1-10	70
4.2 Development of MARS Chemical Fate and Transport Model Variables and Inputs to Simulate Contaminant Transport Phenomena	70
4.2.1 Dissolved and DOC Biodegradation Rate Constant at 20°C	71

4.2.2 Dissolved K_{bio} Temperature Correction.....	71
4.2.3 Sediment Dissolved and DOC Bacteria Density	71
4.2.4 Sediment Solids Bacteria Density.....	71
4.2.5 Solids Biodegradation Rate Constant at 20°C	71
4.2.6 Solids K_{bio} Temperature Correction.....	72
4.2.7 Water Column Dissolved & Dissolved Organic Carbon Bacteria Density	72
4.2.8 Water Column Solids Bacteria Density	72
4.2.9 Downstream Boundary Concentration.....	72
4.2.10 Upstream Boundary Concentration.....	72
4.2.11 Water Column Initial Concentration.....	72
4.2.12 Sediment DOC Koc-Solids Koc Ratio.....	73
4.2.13 Sediment Bed DOC Concentration.....	73
4.2.14 Water Column DOC Concentration.....	73
4.2.15 Water Column DOC Koc-Solids Koc Ratio	73
4.2.16 Chemical Name.....	73
4.2.17 Print Interval	73
4.2.18 Sediment Bed Temperature.....	73
4.2.19 Water Column Temperature	74
4.2.20 Acid Hydrolysis Rate Constant at 20°C	74
4.2.21 Alkaline Hydrolysis Rate Constant at 20°C	74
4.2.22 Hydrolysis Rate Constant Temperature Correction.....	74
4.2.23 Neutral Hydrolysis Rate Constant at 20°C	74
4.2.24 Sediment Bed pH	74
4.2.25 Water Column pH.....	75
4.2.26 Sediment Layer Depth	75
4.2.27 Solids Density	75
4.2.28 Kow-Koc Intercept and Slope.....	75
4.2.29 log Kow.....	76
4.2.30 Sediment Bed Fraction Organic Carbon.....	76
4.2.31 Solids Dependent Partition Parameter	76
4.2.32 Water Column Fraction Organic Carbon.....	76
4.2.33 Chemical Molecular Weight.....	77
4.2.34 Henry's Law Constant	77
4.2.35 Volatilization Option	77
4.2.36 Bed Boundary Condition Scale Factor	77
4.2.37 Bed Boundary Condition Time Series Number	77
4.2.38 Groundwater Flow Scale Factor	77
4.2.39 Groundwater Flow Time Series Number.....	78
4.2.40 Initial Concentrations in Sediment Layers.....	78
4.2.41 Sediment Layer Diffusion Coefficients	78
4.2.42 Water Column-Sediment Interface Diffusion Coefficient.....	78
4.2.43 Sediment Bed Solids Concentration	78
4.2.44 Bed Boundary Condition Time Series Numbers 1-10	79
4.2.45 Groundwater Flow Time Series Numbers 1-10	79
4.3 MARS Chemical Fate and Transport Model Results	79
4.3.1 Chemical Fate and Transport Model Results.....	79

4.4 Conclusions and Recommendations for Future Improvements	81
4.4.1 Conclusions.....	81
4.4.2 Recommendations for Future Improvements.....	83
Chapter 5: Comprehensive Review of MARS Modeling Results and Recommendations	84
5.1 Discussion of Hydrodynamic Model Results	84
5.1.1 Conclusions.....	84
5.1.2 Recommendations for Future Improvements.....	84
5.2 Discussion of Sediment Transport Model Results.....	85
5.2.1 Conclusions.....	85
5.2.2 Recommendations for Future Improvements.....	85
5.3 Discussion of Chemical Fate and Transport Results	85
5.3.1 Conclusions.....	85
5.3.2 Recommendations for Future Improvements.....	86
5.4 Recommendations for Future Model Additions	86
References.....	87
Appendix A: USGS Anacostia River Peak Flows	91
Appendix B: Geochronological Analyses.....	94
Appendix C: Coring Contaminant Concentrations	103
Appendix D: Sediment Geotechnical Analysis.....	107
Vita.....	110

Abstract

The Anacostia Active Capping Project (AACP) is a United States Environmental Protection Agency (EPA) funded initiative to develop and implement, on a field scale, active capping barrier technologies. Overseen by the Hazardous Substance Research Center, South and Southwest (HSRC), the AACP plans to demonstrate the ability of active capping barrier technologies to prevent the migration of contaminants from the sediment bed to the overlying water column of the Anacostia River. The demonstration project will involve the placement and monitoring of four individual types of capping materials (apatite, Aquablok, coke breeze, and sand) and the monitoring of one control (i.e. uncapped) area.

An integral part of this capping/monitoring effort will be the use of the Model for the Assessment and Remediation of Sediments (MARS) to project long term cap stability and effectiveness. Developed by the Electric Power Research Institute (EPRI), MARS allows for the modeling of river hydrodynamics, sediment transport, chemical fate/transport, and contaminated sediment remediation with one stand-alone model. It is the object of this research to not only model river characteristics and cap effectiveness but to also identify those areas of the MARS model which could benefit from revisions to allow for future active capping barrier simulations.

Model projections illustrate the demonstration area as being a zone of sediment deposition during normal flow events. Furthermore, MARS predicts Aquablok and coke breeze as being the most effective capping barriers when considering PAH migration from the sediment column to the overlying water body. Apatite displayed little PAH contaminant retardation as this barrier is being implemented in the AACP in an attempt to precipitate heavy metals from the sediment and pore water.

Chapter 1: Introduction

As the environmental awareness of the world's populace increases, the remediation of contaminants in the environment has become an increasing priority for governments, research institutions, and the general public. Although pollutants may be present in any environmental media (e.g. soil, water, and/or air), contaminated sub-aqueous sediments pose a particular health risk as they serve as a prime pathway for chemical migration from contaminated groundwater to overlying surface waters. Once in these surface waters, the contaminants present an exposure hazard to both local marine life and the human population who uses these areas as a source of recreation.

Remediation of these aforementioned contaminated sediments has historically been a high cost endeavor as the sediments ultimately had to be removed and treated to remove the contaminants of concern. Recently-developed remediation techniques, including traditional sand capping, have provided a cost-effective, alternative means of isolating contaminated sediments from the adjacent water body but questions have been raised as to whether traditional sand caps offer the desired level of risk reduction that more historical remediation measures afforded. As a result, permeable reactive barriers, or "active caps", have been developed as a possible alternative, cost effective technology.

Active capping technologies currently lay at the forefront of contaminated riverine sediment remediation techniques and research. While providing the physical containment of potentially migrating contaminants (and the sediment that contains the contaminants) that more traditional sand caps afford, active caps also allow for an effective, possible low-cost means of providing enhanced isolation and/or treatment of the pollutants in the underlying sediment. Active barriers, though not fundamentally different from sand caps, involve the application of

materials other than inert sand (used in traditional sand capping) to encourage sequestration and/or degradation of the contaminants of concern (COCs). Though currently under-utilized as a contaminated sediment remediation technique, the use of active capping technologies in the field scale demonstrations on the Anacostia River will serve to demonstrate cap placement capabilities and discern the effectiveness of active capping as a viable means of contaminant control and sediment remediation in our waterways.

As active capping holds such promise for future contaminated sediment remediation, it has become imperative to develop a model capable of projecting the effectiveness of these remediation technologies, which can then be verified through monitoring activities. The Model for the Assessment and Remediation of Sediments (MARS), a commercially available modeling tool, offers a compromise between sophistication and simplicity in order provide preliminary assessments of hydrodynamics, sediment transport, and chemical fate and transport without extensive data collection. By allowing for the input of those river and sediment bed characteristics that most influence chemical flux at the sediment-water interface, MARS provides a valuable tool in the design of sediment remediation programs.

The Anacostia River, which flows through the District of Columbia, serves as prime candidate to demonstrate the effectiveness of the MARS package in predicting long term (i.e., time > 1 year) contaminated sediment remediation effectiveness. The Environmental Protection Agency's Hazardous Substance Research Center South/Southwest is currently conducting a demonstration of several active capping barrier technologies in the river to demonstrate, on a field scale, technologies that have proven to be effective in laboratory-scale studies. Furthermore, the river's location in an area of major national significance necessitates that any environmental contamination of the water body is dealt with both effectively and efficiently and

the river's use as a means of recreation for the local populace necessitates that any remediation measures be unobtrusive and enduring.

Such a high profile demonstration dictates that extensive measures be in place to ensure both the longevity and effectiveness of such a study. With the use of the MARS, it is hoped that a comprehensive, long-term study of the Anacostia Active Capping Project (AACP) will be available for the first time.

1.1 Anacostia River Demonstration Site Description

The Anacostia River, whose two major tributaries originate in Maryland's Montgomery and Prince George's Counties, flows through Washington, D.C. and serves as a major tributary to the Potomac River. Influenced by the tidal fluctuations of the Chesapeake Bay, the Anacostia is not a true river but rather an estuary of the Chesapeake Bay system (Schultz, 2001).

The Anacostia itself is primarily a result of the overland drainage of two watershed areas known as the Northeast and Northwest Branches, respectively. These drainage areas (see Figure 1.1) constitute approximately 73% of the total Anacostia watershed and combined amount to 129 mi² of drainage area (Northeast Branch, 76 mi²; Northwest Branch, 53 mi²) (Schultz, 2001). The two branches converge near Bladensburg, Maryland and the Anacostia continues on for 8.4 mi from this point in a southwesterly direction through the District of Columbia (Schultz, 2001). Flowing through the heart of Washington, it is estimated that over 800 000 people reside within the defined boundaries of its watersheds (Warner et al., 1997 from Schultz, 2001).

Located within the city limits of one of the United States' most urbanized areas, the Anacostia serves as a particularly hazardous potential pathway for human exposure to any of a myriad of contaminants. The population density alone of the area adjacent to the river warrants considerable environmental remediation efforts. However, in light of recent contamination

studies, the exact extent to which the river is contaminated has become a much more well-known and well-understood fact. The Anacostia has previously been listed as one of the ten most polluted rivers in the United States (Government of the District of Columbia, 1998 from Katz, 2000) and has been determined to be one of the most polluted water bodies within the Chesapeake Bay system (Syracuse, 2000 from Katz, 2000). Such a level of contamination, coupled with the river's presence in such a populated area, has proven to be the driving factors behind the recent push to remediate the Anacostia.

Flowing through such a heavily urbanized area, the Anacostia River serves as a prime candidate for a field scale demonstration of active capping technology. The sediments of the capping demonstration area, seen in Figure 1.2, are subject not only to point sources of pollution such as combined sewer overflows but is also contaminated by urban storm/melt water runoff and contaminants originating from historic military and industrial sites situated along the river's banks. While pollution sources are distributed along the entirety of the Anacostia River in this area, the initial demonstration site lay between the Capitol and Pennsylvania Ave. Street Bridges along the northern shore of the Anacostia, southwest of the Washington Navy Yard. The sediments in this area are subject to much the same contamination as the river itself and are known to contain fairly high levels of the various species of contaminants, particularly heavy metals, polychlorinated biphenyls (PCBs), and polynuclear aromatic hydrocarbons (PAHs) (HSRC, 2004).

The demonstration area has historically displayed high levels of heavy metals, as well as elevated measures of both PCBs and PAHs (see Appendix C). Severn Trent Laboratories (STL) has conducted full chemical and metal analyses on core samples collected by Horne Engineering



Source: <http://www.mdsg.umd.edu/CQ/V02N2/watershed.gif>

Figure 1.1: Anacostia Watershed

Services, Inc. (HES) and EA Engineering, Science, and Technology (EA). Based upon these analyses, all modeling efforts were determined to focus on the chemical migration and capping of a specific polycyclic aromatic hydrocarbon (PAH), phenanthrene, due to its projected, relatively rapid movement through sediment columns and traditional sand caps.

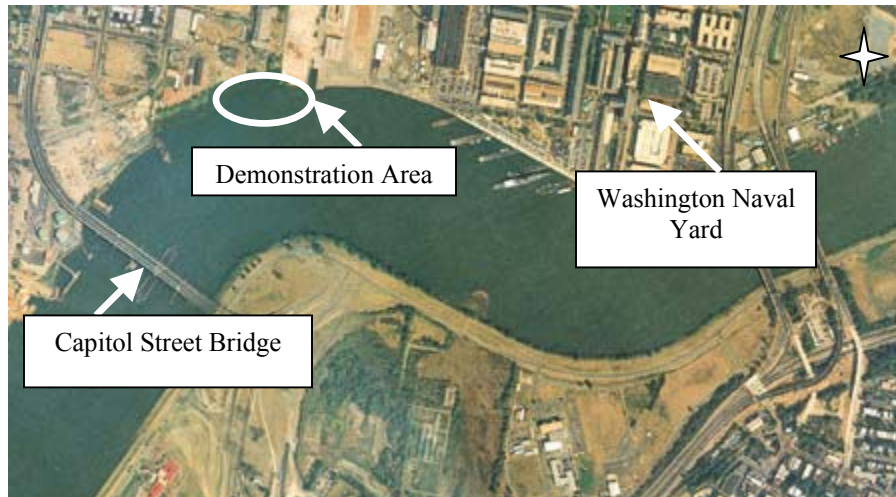


Figure 1.2: Reference Map

1.2 HSRC Anacostia Remediation Effort

The Hazardous Substance Research Center/South & Southwest (HSRC/S&SW), one of five such research centers located throughout the United States, is funded through grants from several agencies and institutions - including the United States Environmental Protection Agency (EPA) and the U.S. Department of Defense - to develop innovative solutions to hazardous substance management (www.hsrc.org). Focusing primarily upon the remediation of contaminated sediments, HSRC/S&SW is in essence a consortium of five universities and is led by Louisiana State University (LSU). One of the current research objectives of the center is to demonstrate, on a field scale, the effectiveness of active capping barrier technologies.

While traditional sand capping is a fairly well understood technique for managing sub-aqueous contaminated sediments, there have been few instances where “reactive” materials were used in cap construction to chemically or physically isolate migrating contaminants.

HSRC/S&SW, through the Anacostia Active Capping Project, will attempt to prevent the migration of the COCs, particularly PAHs and PCBs, from the sediment bed into the overlying water column by allowing the contaminants to flow through capping barriers constructed of various materials whose physical and/or chemical properties are favorable to the sequestration of

the contaminants. Of particular future interest to the Center is the effectiveness of ¹Aquablok™ (a gravel core with a clay covering used to manage groundwater seepage and contaminant advection), ²zero-valent iron (used to encourage metals reduction and the dechlorination of chlorinated organic compounds), ³apatite (used to encourage metals reduction and sorption of contaminants), ⁴BioSoil™ (used to encourage anaerobic degradation and dechlorination of contaminants), ⁵OrganoClay sorbent (used to manage contaminant advection and diffusion), and ⁶coke breeze (used to encourage contaminant sorption) (www.hsrb-ssw.org).

As of the summer of 2004, four active capping barriers composed of sand, Aquablok™, coke breeze, and apatite, had been placed in the Anacostia River. Long term monitoring will be used to gauge the actual effectiveness of the capping barriers on the migration of PCBs, PAHs, and heavy metals.

1.3 Literature Review

1.3.1 Review of Previous Anacostia River Hydrodynamic Studies

Despite the Anacostia River's presence in the nation's capitol, there appears to be only limited information available concerning the river's hydrodynamic features and history. Repeated requests to governmental agencies and independent research firms revealed that significant data concerning typical hydrologic flows was limited at best. However, some background data was compiled from two research reports concerning the Anacostia River - from its origin to its confluence with the Potomac River (Schultz, 2001; Katz et al., 2000) - and limited information on gauge heights and flow volumes was available from the United States Geological Survey (USGS).

Predicted flow velocities were typically less than 0.5 m/sec for the period of 1988 through 1990 and a range of measured velocities ranged from 0 to 0.3 m/sec during non-storm

periods of the same time span (Schultz, 2001). Furthermore, Schultz also concluded that simulated flow velocities in the Anacostia River are lowest in the river segment downstream of the 11th Street Bridge, which is that stretch of river being used as the demonstration site for the AACP (see figure 1.3). Approximate median flow velocities in this area are predicted to be 0.03m/sec (Schultz, 2001). Schultz (2001) used the Tidal Anacostia Model, originally developed by the Metropolitan Washington Council of Governments, to predict flow velocities in the Anacostia River.

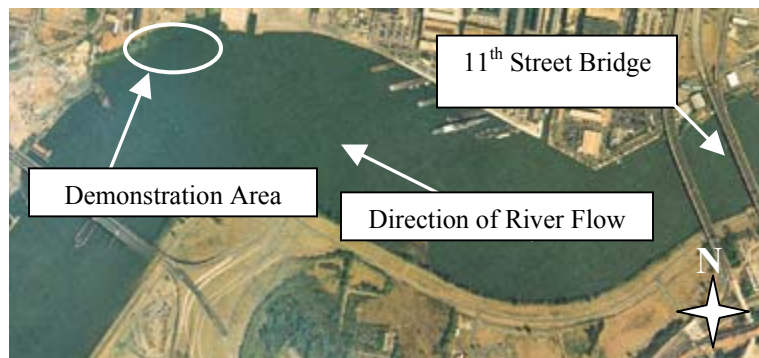


Figure 1.3: Region of Low Flow Velocities

A study by Katz et al. (2000) employed the use of a fixed point Acoustic Doppler Current Profiler (ADCP) and measured flow velocities in the Anacostia River south of the Capitol Street Bridge on the order of 0.1 m/sec. Furthermore, the report concluded that the Anacostia River displays a fairly vertically homogenous velocity profile near the AACP demonstration area. The vertically homogenous velocity profile suits the MARS hydrodynamic model runs well due to the internal model assumption of vertically averaged water velocities (Jain, 2003).

While both simulated and field-gathered velocity measurements indicated a region of particularly low flow velocities in the vicinities of the Capitol and 11th Street Bridges, these velocities were based upon the approximate river discharge of 4.94 m³/sec during the time of

Katz's study (Katz et al., 2000). Little to no information was available regarding low frequency storm events and their effects on the Anacostia River's hydrodynamics.

1.3.2 Review of Previous Anacostia River Sediment Transport Studies

Schultz (2001) uses the EPA's Water Analysis Simulation Program (WASP) in an effort to quantify Total Suspended Solids (TSS) loadings in the river. Schultz (2001) study predictions display peak storm water column TSS measurements in the range 150 to 250 mg/L for all ranges of sediment sizes (fine clays to sand grains) and typical, non-storm TSS loads of 5 to 30 mg/L (Schultz, 2001). Furthermore, annual sediment load estimates for the lower Anacostia River illustrate a range of loads from 46 000 tons (Warner et al., 1997 from Schultz, 2001) upwards to 138 000 tons (Century Engineering, 1981 from Schultz, 2001).

Actual field measurements by Katz (2000) of suspended particles in the Anacostia River appear consistent with the predicted values of the WASP model. The range of particle sizes of suspended solids in various river samples was consistently below 30 μ m (>85% total suspended solids were smaller than 30 μ m). Additionally, TSS concentrations associated with a river discharge of 4.94 m³/sec in the vicinity of the demonstration area were shown to range from 10 to 12.5 mg/L and to be vertically homogenous throughout water column (Katz et al., 2000).

1.3.3 Review of Previous Anacostia River Chemical Fate and Transport Studies

There have been no relevant studies concerning the in-situ migration of contaminants through the Anacostia River sediment bed.

1.3.4 Review of Alternative Predictive Hydrologic Modeling Software Packages

While there exists numerous hydrologic modeling software packages, the most commonly employed include the U.S. Army Corps of Engineers (USACE) Hydrologic Engineering Center's (HEC) series of programs. The most recent release, River Analysis System

(HEC-RAS), is an effective hydrodynamic model. HEC-RAS is able to simulate overbanking, construct flood-rating curves, predict bridge scour, and produce three-dimensional representations of river systems. HEC-RAS is a superb modeling tool for predicting near all aspects of a hydrologic event or simulating a typical river discharge (Haested et al., 2003).

Despite the effective modeling capabilities of the HEC-RAS system, MARS does possess several advantages over the ASCOE model. The most glaring advantage of the MARS model over the HEC-RAS system is the comprehensive structure of its modeling packages that allows for consecutive simulations of hydrodynamics, sediment transport, chemical fate and transport, and remediation measures. While the effectiveness of the Corps' model is undisputed, MARS' ability to model contaminated sub-aqueous sediments from hydrodynamics to remediation renders it favorable for application to the AACP. The HEC-RAS model was used, however, in the development of several of the required inputs for the MARS hydrodynamic model.

The Tidal Anacostia Model comprises the hydrodynamic component of the TAM/WASP modeling framework. Developed for the Metropolitan Washington Council of Governments, the TAM model has been used effectively by the ICPRB to predict various hydrologic aspects of the Anacostia River for input into the WASP model to determine sediment transport within the river system (Schultz, 2001). As previously mentioned, the comprehensive modeling offered by the MARS model gives it a distinct advantage for use in the Anacostia Active Capping Project. Results from the TAM model (Schultz, 2001) will be used, however, to verify applicable MARS hydrodynamic model predictions.

1.3.5 Review of Alternative Predictive Sediment Transport Modeling Software Packages

The EPA's Water Analysis Simulation Program is one of the most relevant sediment transport models available and a modified version (to include river flow velocity induced

deposition and resuspension of solids) was employed by ICPRB to model the sediment transport properties of the Anacostia River (Schultz, 2001). As previously mentioned, the comprehensive modeling offered by the MARS model gives it a distinct advantage for use in the Anacostia Active Capping Project. Results from the WASP model (Schultz, 2001) will be used, however, in the development of several of the required inputs for the MARS sediment transport model.

1.3.6 Review of Alternative Predictive Chemical Transport Modeling Software Packages

The HSRC Capping Design Model is one of the most relevant predictive chemical transport modeling software packages available. Developed by the HSRC/S&SW, this web-based model is used to design and predict the overall remediation effectiveness of capping barriers as they relate to sub-aqueous contaminated sediments (www.capping.hsrb.lsu.edu). Unlike MARS, however, the HSRC model projects contaminant migration at a single point instead of allowing for the modeling of vertical chemical migration over a wide spatial area and is incapable of modeling hydrodynamics or sediment transport.

1.3.7 MARS Model Hierarchy

The MARS modeling structure is essentially a three tiered model and is configured in the following sequential order: ¹hydrodynamics, ²sediment transport, and ³chemical fate and transport. MARS allows for several daughter runs below a single parent model simulation (i.e. three sediment transport simulations using the same hydrodynamic model projection) and, as such, allows for efficient simulations of varying river, sediment, or chemical properties. The MARS modeling hierarchy can be viewed in Figure 1.4.

1.4 Research Objectives

The focus of this research is to determine the overall effectiveness of the selected active capping barrier technologies over the lifespan of the cap as well as to predict the geotechnical

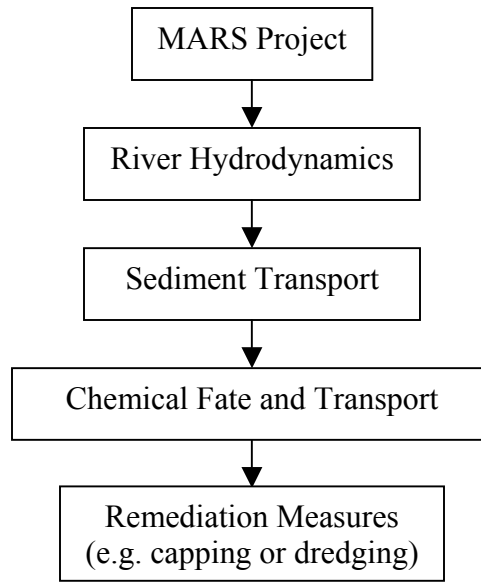


Figure 1.4: MARS Hierarchy

stability of the capping materials when exposed to storm event flow conditions. In particular, the objectives of this research are as follows:

1.) To evaluate a commercially available model for the design and evaluation of sediment remedial approaches without extensive site specific data, including the following:

A.) To conduct sensitivity analyses on all significant variables to ensure the validity of model results as well as verifying model predictions against available field data, literature data, and additional applicable models.

B.) To determine the geotechnical stability of the cap materials when subjected to typical and extreme river hydrodynamic forces. Geotechnical stability analyses will involve subjecting 6-inch caps to low return frequency storm events (5, 10, 25, 50, and 100 year) to discern if any significant erosion of the capping material will occur.

C.) To investigate the significant factors and processes associated with field scale active capping projects, including general river hydrodynamics and sediment transport phenomena in tidally-influenced estuary systems; chemical fate and transport of polynuclear aromatic

hydrocarbons in contaminated porous media; and isolation/treatment of PAHs through the use of active capping barriers. Simulations will be performed using each of the active capping materials in order to develop a basis of comparison to determine overall cap effectiveness in regards to contaminant isolation/treatment as well as to determine if there is, as expected, an increase in pollutant treatment and isolation as compared to more traditional sand caps (i.e., base case).

D.) To determine possible revisions to the MARS program to facilitate further use and development of the model. These revisions include, but are not limited to, illustrating model flaws and limitations, providing suggestions for generic improvements to aid in modeling endeavors, and providing a comprehensive list of PCB congeners and their associated properties for incorporation into future MARS editions.

2.) Predict performance of permeable reactive capping barriers using this approach.

Chapter 2: Hydrodynamic Modeling of the Anacostia River

The hydrodynamic modeling portion of the Model of the Assessment and Remediation of Sediments (MARS) is based upon an enhanced version of a previous HydroQual modeling package, the ECOM hydrodynamic model (Jain, 2003; Blumberg and Mellor, 1980). A key element of these revisions to ECOM was modifications made to ensure that MARS could handle the vigorous calculations necessary to simulate long term hydrodynamic events. In a quest to effectively balance computational time with model accuracy, certain simplifications are assumed, including a vertically homogenous water column (Jain, 2003).

The general governing equations for the hydrodynamic model are (Jain, 2003):

$$\frac{\partial \eta}{\partial t} + \frac{\partial V_x D}{\partial x} + \frac{\partial V_y D}{\partial y} = 0 \quad (\text{Equation 2-1})$$

$$\frac{\partial V_i D}{\partial t} + \frac{\partial V_i^2 D}{\partial x} + \frac{\partial V_x V_y D}{\partial y} - f V_i D + g D \frac{\partial \eta}{\partial x} - \tilde{F}_i = -\tau_i^b \quad (\text{Equation 2-2})$$

Where: V_i = vertically averaged current velocity in i-direction (length/time); will be either x or y
 D = flow depth (length)

t = time

V_x = vertically averaged current velocity in x-direction (length/time)

V_y = vertically averaged current velocity in y-direction (length/time)

f = Coriolis parameter (1/time)

g = gravity (9.81 m/sec²)

η = surface elevation (length)

\tilde{F}_i = eddy viscosity effects in i-direction (length²/time²); will be either x or y direction

τ_i^b = bottom shear stress in i-direction (length²/time²); will be either x or y direction

2.1 Description of Grid Generation for MARS Model

The initial stage of the MARS modeling package requires the input of a bitmap or jpeg image of the region of interest into the software. Two reference points are chosen from the input image and are assigned both x and y locations by the user. These reference points are typically established with Point 1 having measures of $x = 0\text{m}$ and $y = 0\text{m}$ and Point 2 having the

appropriate meter distances from reference point 1. By inputting these reference points and their associated distance values, the user provides a frame of relative reference from which the model can establish the size proportions of segmentation grid cells.

From this image, river shorelines and upstream and downstream boundaries are established using features of the MARS package. These boundaries will serve to limit the extent of river flow as the model is unable to simulate flow beyond these boundaries. A segmentation grid is then installed by the model upon user designation of number of grid cells. For purposes of this modeling effort, grid cells were based on 10 row, 30 column format. MARS then fits the appropriate number of grid cells to the defined boundary conditions and adjusts the size of the cells to represent a finer grid at the inside of river bends. A 10 row, 30 column format was chosen due to the fact that model execution time is directly proportional to grid size. The segmentation grid can be seen in Figure 2.1.

2.2 Description of MARS Hydrodynamic Model Variables and Inputs

The MARS modeling package requires the input of 15 user-provided variables and/or constants to efficiently simulate hydrodynamic flow events. While all inputs are accompanied with default values and limiting ranges of possible values, the accuracy of these inputs is vital to the successful modeling of a flow event. Due to the varying nature of certain river and flow event characteristics, sensitivity analyses should be conducted on those variables deemed to have the most influence on model outputs. These analyses, along with model results, will be discussed in depth in the Results section of this chapter.

2.2.1 Length of Simulation

The Length of Simulation (LOS) input determines the time span for which the hydrodynamic model will be executed. Equipped with a default value of 365 days, this value is

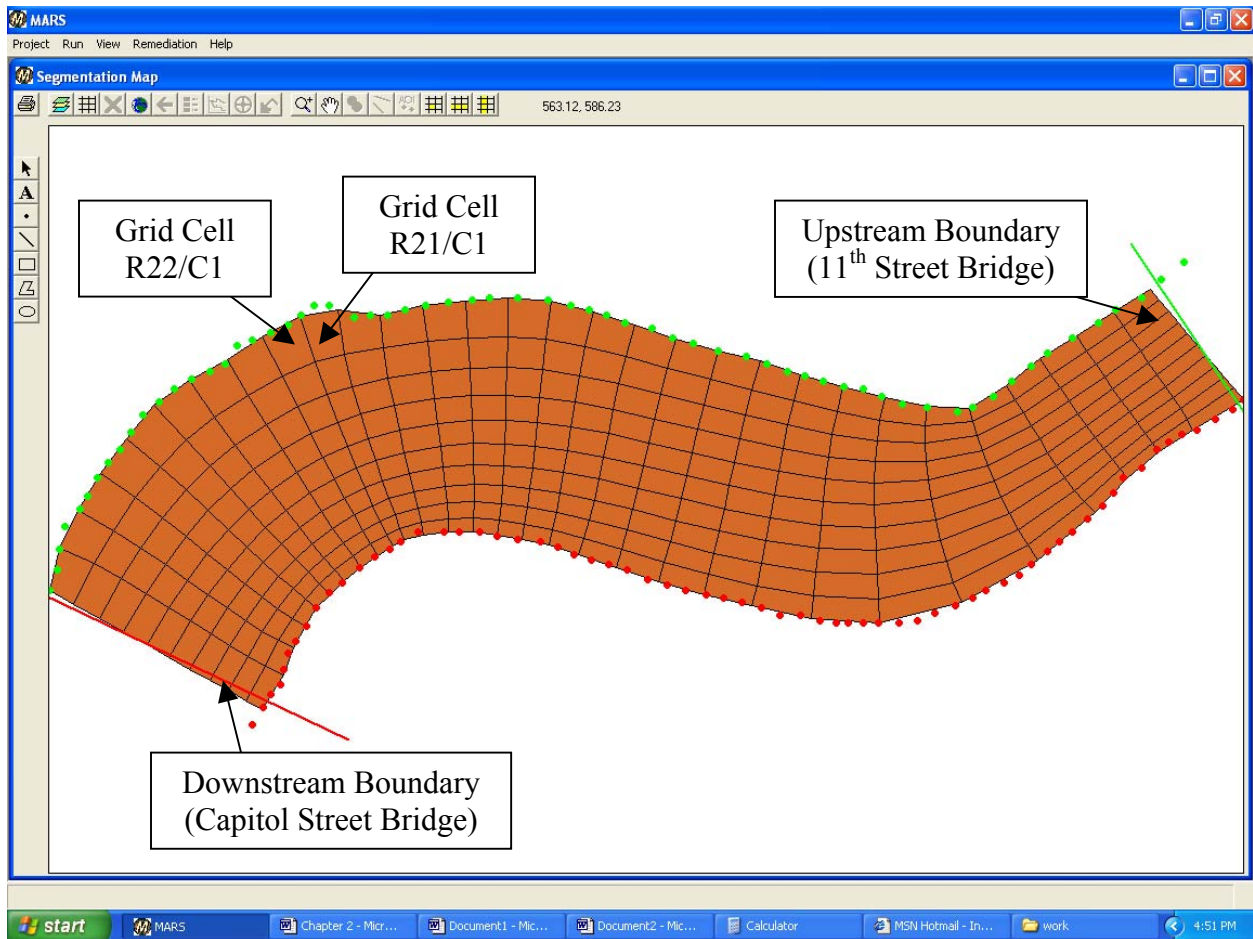


Figure 2.1: Mars Segmentation Grid

determined solely by user need and requires a minimum input of 1 day. While model computation time is directly proportional to this variable, it is suggested that all sensitivity analyses have an adjusted LOS to reflect the absolute minimum amount of time required to determine the influence of the particular variable of interest (Jain, 2003).

2.2.2 Print Interval

Basically, the print interval input is the reporting interval for the model. Model results will be displayed for each interval possible given the specified LOS. For instance, a model run with a stipulated LOS of ninety days and a reporting interval of thirty days will allow for three data points to be displayed in the model results (one data point at each the thirty, sixty, and

ninety day times). As with the LOS, computational time is directly related to the print interval input selected. It should be noted however, that the model requires that there be at least two full reporting intervals within a given length of simulation. Failure to do so will result in a model failure.

The default value for the print interval is set at thirty days and there exists no upper bound on value. The minimum value for print interval is set at 0.041667 days, or 1 hour (Jain, 2003).

2.2.3 Dimensionless Drag Coefficient

The dimensionless drag coefficient input (C_f) is a user-supplied value which is used to establish the bottom shear stresses exerted by water flow on the sediment column at the sediment-water interface through the quadratic stress law. The MARS model supplies a default dimensionless drag coefficient of 0.0025 and sets upper and lower bounds of 0.03 and 0.0025, respectively. Typical field values for C_f range from 0.0025 to 0.0040 (Martin and McCutcheon, 1999). Development of the individual boundary shear stresses, in both the X and Y directions, exerted on the sediment at the sediment-water interface is as follows (Jain, 2003):

$$\tau = \rho C_f Q V \quad (\text{Equation 2.2-1})$$

Where: ρ = water density (mass/length³)

V = water velocity (length/time)

C_f = dimensionless drag coefficient

$Q = (V_x^2 + V_y^2)^{0.5}$

V_x and V_y represent water velocities in the x and y directions, respectively

2.2.4 Horizontal Dispersion Parameter

The horizontal dispersion parameter is employed to influence water column dispersion and is set at a default value of 2 and requires a minimum value benchmark of 0 (there is no upper bound for the input) (Jain, 2003). Sensitivity analyses involving this parameter display an

apparent effect of the parameter on the velocity profile of the river, across the direction of flow (i.e., from bank to bank). The particular default value for the horizontal dispersion parameter was chosen based on slug tracer studies conducted on the Hudson River (Hellweger, 2003).

2.2.5 Tidal/River Variable

The Tidal/River constant allows a user to dictate whether the river of interest is influenced by local tidal fluctuations or if the river is simply free flowing. A selection of the number 1 allows for all model runs to function as if the river is tidally influenced. These simulations require further input concerning tidal amplitudes and tidal periods in order to effectively model the associated hydrodynamics. A selection of the number 2 indicates that MARS will model the river of interest as a non-tidally influenced water body and requires the input of information regarding the depth-flow rating curve/function in order to effectively simulate river flow stages and events (Jain, 2003).

2.2.6 a, b, and c in the Depth-Flow Function

The Depth-Flow equation is as follows (Jain, 2003):

$$D = aQ^b + c \quad (\text{Equation 2.2-2})$$

Where: D = average depth of flow at downstream boundary (meter)

a = empirical coefficient

Q = flow rate (meter³/second)

b = empirical coefficient

c = height of dam/structure (meter)

The constants *a*, *b*, and *c* in the depth flow function are used by the hydrodynamic model to regulate water depth at the downstream boundary as a function of flow rate for non-tidally influenced rivers. *a* and *b* are both empirical coefficients and have designated default values of zero for both. The lower bound for *a* is defined as zero (there is no upper bound) and the range of acceptable values for *b* are 0.1 to 0.7. It should be noted that the default value for *b* (0) is not

within the acceptable range and, as such, a satisfactory value must be entered for the b input to ensure model operation (Jain, 2003).

While there exist field-determined values for these inputs for individual rivers, it is advisable to develop rating curves (flow depth versus discharge) (Thomann and Mueller, 1987; Chapra, 1997; Schnoor, 1996; USEPA, 1988; all from Jain, 2003). Hydrodynamic modeling packages such as HEC-RAS can be used for developing river rating curves for flow events to be used as MARS model inputs. Results from these modeling softwares can be exported to statistical/spreadsheet programs in order to impose a best-fit exponential line to garner the required depth-flow rating curve and associated empirical coefficients. Particular uses and development of these rating curves will be discussed later in this chapter.

The input c is used to regulate depth of flow as it relates to a dam or other obstruction present in the river system and has an established default value of zero meters, a lower bound of zero meters, and no upper bound. To represent a river system having no dam, one need only set the c input value to 0.

2.2.7 12-hour and 24-hour Tidal Phase

The 12-hour and 24-hour tidal phases are constant inputs which are used to adjust MARS hydrodynamic model runs to better simulate observed field tidal conditions. These phase shifts are used to offset the occurrence of the 12-hour and 24-hour tidal peaks from the beginning of the model run (time = 0) to that point in time at which the observed tidal crests are expected to occur. These inputs are measured in units of minutes and are assigned default values of 0. The upper and lower bounds of accepted input values for both parameters are 360 and 0 minutes, respectively (Jain, 2003).

2.2.8 12-hour and 24-hour Tidal Amplitudes

23.93- hour tidal period amplitudes, respectively. The tidal amplitudes, for model purposes, are defined as the linear distance between the top of the cresting elevation of the tidal cycle and the mean water elevation. Both inputs are assigned a default value of zero meters by the model and have no model limitations concerning maximum input (Jain, 2003).

Extended communications with MARS programmers have illustrated that these inputs are used to vary the water surface elevation at the downstream boundary as a function of time and input amplitude. The use of two amplitude inputs allows for the specification of two tidal waves (12- and 24-hour), whose sum is then employed as the downstream water surface elevation. Model manipulation does allow for a field observed tidal amplitude to be input for the 12-hour amplitude, while the 24-hour amplitude, in this particular case, should be set to zero (Hellweger, 2003).

2.2.9 Depth Shift

The depth shift input parameter allows for the adjustment of the downstream water elevation if the bathymetry used to establish water elevations is different from the observed mean water elevation at this boundary. The default value for this parameter is set at zero meters and there is no maximum or minimum value (Jain, 2003).

2.2.10 Water Column Depth

Water column depths are input into the MARS hydrodynamic model as spatial variables and are allowed to vary between, but not within, grid cells. Once a segmentation grid is established for a particular model run, user input defines all initial water column depths, which are then adjusted during model computations to accommodate both applicable flow rates and input rating curves or specified tidal influences. Model-calculated water depths are subsequently

recorded as “WC Depth Used” and are accessible at later times to the user. Default water column depths are set at 1 meter and are allowed to range to any value above zero (Jain, 2003).

Despite MARS’ capabilities, the model is unable to simulate periodic overbanking of a river. While individual grid cells can be established to exhibit no water flow (by having their water column depth set to 0 m), MARS is incapable of establishing a flood plain adjacent to the river if interest. Furthermore, grid cells exhibiting a depth of flow of less than 0.25 m will have their flow depth adjusted by the hydrodynamic model at the time of execution (Jain, 2003). This feature will have no impact on Anacostia simulations as all water depths are at least 1 m.

2.2.11 Flow Rate

River flow rates in the MARS hydrodynamic model are temporal variables that are specified by the user before model execution and serve as time-variable upstream boundary conditions within the framework of the model. The default value for rates of discharge is set at 100 m³/sec and the model has no upper bound restraining user input of this parameter. For inputting purposes, data sets in tab-delimited formats can be imported to expedite the flow rate input process (Jain, 2003).

All flow rate inputs used for model computations are divided into statistically segmented “flow bins” for ease of calculation. Capable of constructing up to 25 such bins, MARS correlates the number of statistical bins to the length of the flow record input into the model for simulation, with longer flow records resulting in more flow bins. Within each flow bin, a mean flow value is determined to represent all individual values in the associated bin for subsequent model calculations. As flow rates increase, the resolution of the corresponding bins increases (Jain, 2003).

It is also of vital importance that upstream boundaries be established at a sufficient distance from downstream boundaries to preserve accuracy in hydrodynamic model results. At execution, volumetric water flows are distributed at the upstream boundary according to established water column depth in an effort to conserve a uniform lateral velocity distribution. As a direct result, model results near upstream boundaries do not display a high degree of accuracy as the model will not have had an opportunity to correct flow rates and corresponding velocities as river features would naturally dictate. While this event is corrected as a function of distance from the upstream boundary, it is advisable to take note of this model characteristic (Jain, 2003).

2.3 Development of MARS Hydrodynamic Model Variables and Inputs to Simulate Anacostia River Flow Events

The model parameters employed in the hydrodynamic modeling of the Anacostia River were developed from both historical and field data as well as from literature sources on the subject. All parameters were selected on the basis of inputting into MARS the most accurate information available to ensure the proper representation of river characteristics in all simulations as well preserving the quality of all model predictions. All hydrodynamic model parameters were selected based upon the premise of ultimately imposing a steady state (SS) volumetric flow through the river for all flow event scenarios, as accurate data on storm-event flow volumes is near non-existent for the Anacostia. All model simulations for the Anacostia project reached steady state values within the first reporting interval (30 days).

2.3.1 Length of Simulation

The length of time input parameter for all hydrodynamic model runs was established at 365 days. While such a length of time may seem excessive for SS flow scenarios, the hydrodynamic LOS serves as a limiting factor for all subsequent sediment and chemical

fate/transport runs as these subsequent model executions can not be computed for time periods which exceed the hydrodynamic LOS.

2.3.2 Print Interval

The print interval input parameter for all hydrodynamic model simulations was established at 30 days. Such a reporting interval allows for the model production of 12 data points, or roughly one reference value per month.

2.3.3 Dimensionless Drag Coefficient

The dimensionless drag coefficient parameter for all hydrodynamic model runs was set to 0.0025, the default value provided by MARS. The default value was selected for use based on the limitation of an absence of reliable flow velocity data from which calculations could be made. Results from sensitivity analyses will be provided in the conclusion of this chapter.

2.3.4 Horizontal Dispersion Parameter

The horizontal dispersion parameter for all hydrodynamic model runs was established at the model default value of 2.00. After preliminary experimentation, it was determined that the input value of 2.00 provided the most realistic representation of field measured horizontal river flow velocity profiles. Higher values for this parameter resulted in extreme shoreline-to-shoreline velocity profiles that did not accurately represent typical river hydrodynamics.

2.3.5 Tidal/River Variable

The tidal/river variable for all hydrodynamic model runs was set to represent a non-tidal river system, despite the Potomac River's obvious tidal effects on the Anacostia. The non-tidal option was chosen due to the model's intrinsic method of evaluating such tidal influenced hydrodynamic features as flow depth and velocity. The MARS hydrodynamic model, by default, establishes an area of no tidal influence at the defined upstream boundary of the river system and

interpolates tidal effects at all points between the upstream and downstream constraints. In order to reach regions of the Anacostia River devoid of tidal influence (i.e. extend the model further upstream), the model-produced segmentation grid would have been of such size that model computation time and grid cell precision (to represent the capping demonstration area) would have been severely sacrificed.

2.3.6 a, b, and c in the Depth-Flow Function

All variables in the depth-flow function were established using a combination of Log-Pearson Type 3 distribution statistical analyses of historic Anacostia volumetric flows as well as model predictions of HEC-RAS software for low-frequency storm events in this geographic area.

Initial development of variables for the depth-flow function required historical discharge rates for the Anacostia River. While no data exists for the river stretch containing the demonstration capping area, the United States Geological Survey's (USGS) river monitoring stations had collected peak flow data for a period of 65 years for the two branches of the river upstream from the Capitol River Bridge (See Appendix A) at USGS stations 01649500 and 01651000 (See Appendix A). After statistical analysis to project low-frequency storm event flows, these peak flow events (one per branch) were combined to produce a combination flow and adjusted by a factor of 1.322 to account for overland flow contributions to the Anacostia along the river stretch from the two upstream branches to the demonstration area (EA, 2003).

It was determined that model projections of river hydrodynamics would be made for typical flow years as well as for projected flows associated with 5, 10, 25, 50, and 100 year storm events. Calculations for storm event flows had to be produced using a Log-Pearson Type 3 statistical analysis of previous Anacostia peak flow events. Statistical analyses were made using the following equations (Bedient and Huber, 1982):

$$y^t = \text{Mean.Log.Flow} + K \cdot \text{Std.Log.Deviation} \quad (\text{Equation 2.3-1})$$

Where: y^t = power to which 10 is raised to compute storm-event discharge

K = Frequency Factor and is determined by Return Interval and Skew Coefficient, C_{s2}

Mean Log Flow (based on peak events) = 2.326 (based on 65 year record)

$$C_{s2} = \left(1 + \frac{6}{n}\right) \cdot C_{s1} \quad (\text{Equation 2.3-2})$$

Where: n = Number of independent samples

$$C_{s1} \equiv \hat{g} = \frac{n}{(n-1)(n-2)} \cdot \frac{\sum (x_i - \bar{x})^3}{S_x^3} \quad (\text{Equation 2.3-3})$$

$$S_x^2 = \frac{1}{(n-1)} \sum_{i=1}^n (x_i - \bar{x})^2 \quad (\text{Equation 2.3-4})$$

Where: x_i = individual year peak discharge measurement (length³/time)

\bar{x} = average peak discharge measurement (length³/time)

Using Microsoft Excel, C_{s2} was found to equal 1.065 and S_x was found to have a value of 0.282. Using the K table provided in Bedient and Huber the following y_t , Q_t , and $Q_{t\text{-corrected}}$ were determined:

Table 2.1: Corrected Storm Discharge

Return Interval (years)	K Value	y_t	Q_t (cms)	Q_t corrected by 1.322 (cms)
5	0.750	2.538	345	456
10	1.341	2.705	507	670
25	2.058	2.907	808	1068
50	2.570	3.052	1126	1489
100	3.064	3.191	1553	2053

Where: $Q_t = 10^{y_t}$

Due to possible river overbanking, it was necessary to again adjust storm event discharge values to compensate for river flow not carried by the channel, as MARS does not easily allow for overbanking scenarios. HEC-RAS was used to determine the amount of discharge conveyed by the defined river boundaries (during normal flow events) during severe flooding. For this purpose, the defined river boundaries are the boundaries that carry the river flow during normal flow events.

Using topographic data obtained from the District of Columbia government, a HEC-RAS model of the Anacostia River demonstration area was produced. Analysis of resultant data led to a depth-flow function (i.e. rating curve) of $y = 0.3334x^{0.2100}$ ($a = 0.3334$, $b = 0.2100$, $c = 0$). The rating curve for normal flow events was found to be $y = 4.22x^{0.1}$. The difference in rating curves between normal and extreme events is expected (Singh, 1992). Furthermore, predicted discharged rates carried within the defined river boundaries (shorelines under typical flow conditions) were corrected by a volume of 60 m^3 to account for differences in volumetric flow attributed to tidal fluctuations and used as input values for MARS discharge rates were as follows:

Table 2.2: Channel Conveyances

Return Interval (yr)	5	10	25	50	100
HEC Q_{input} (cms)	456	670	1068	1489	2053
Channel Q_{conveyed} (cms)	410	561	767	919	1080
Tidal Correction (m^3)	60	60	60	60	60
MARS Q_{input} (cms)	470	621	827	979	1140

2.3.7 12-hour and 24-hour Tidal Phase

The 12-hour and 24-hour tidal phase input parameters were set to 0 for all hydrodynamic runs as the river was established to be non-tidally influenced for modeling purposes.

2.3.8 12-hour and 24-hour Tidal Amplitudes

The 12-hour and 24-hour tidal amplitude input parameters were set to 0 for all hydrodynamic runs as the river was established to be non-tidally influenced for modeling purposes.

2.3.9 Depth Shift

The depth shift input parameter was established at 0 meters.

2.3.10 Water Column Depth

All input water column depths were input into the model once a reasonable segmentation grid had been generated. Input for the depth parameters was taken from previous SPAWAR bathymetric surveys of the Anacostia River (Katz et al., 2000) and checked against field gathered information from the demonstration site (Earth Resources Technology, Inc., 2003).. Initial depths were calculated to represent mean water depths at average flow rate over a twenty-four hour period to compensate for the model simulating a non-tidally influenced river.

2.3.11 Flow Rate

Volumetric flow rate input parameters were established using results from preliminary HEC-RAS model simulations. Since MARS has no features specifically designed to handle river overbanking, HEC-RAS was used to determine channel conveyance during low frequency storm events. The computed channel conveyance was then input into the MARS model to represent the flow conditions associated with each storm. The actual values employed in model computations can be found in Table 2.2.2 as MARS Q_{input} .

2.4 MARS Hydrodynamic Model Results

Hydrodynamic model results were checked for accuracy using two methods. Initial verifications were made using a mass balance to ensure that volumetric discharge was conserved

throughout model computations between upstream and downstream boundaries. Model results were then compared to HEC-RAS predictions, particularly downstream flow velocities as these values will directly influence subsequent sediment transport and chemical fate/transport models through their effects on sediment bed deposition/erosion.

2.4.1 Hydrodynamic Model Results

Hydrodynamic results for the downstream boundary (Capitol Street Bridge) and for the capping demonstration area (segmentation grid cells R21/C1, R22/C1) can be found in the subsequent tables, Table 2.3 through 2.8. Table 2.9 is a comprehensive listing of flow velocities during normal flow conditions and 5, 10, 25 50, and 100-year storm events.

Table 2.3: Typical Year Flows

Column Number	Grid Cell Width	Flow Velocity
(Row 30)	(meters)	(m/s)
1	45.56	4.00E-02
2	41.37	3.55E-02
3	38.84	3.29E-02
4	36.58	3.07E-02
5	34.5	2.89E-02
6	32.59	2.71E-02
7	30.83	2.54E-02
8	29.24	2.38E-02
9	27.79	2.22E-02
10	25.74	2.09E-02
Sum = 343		
Mass Rate In (cms):	65.00	
Mass Rate Out (cms):	65.00	
Width Avg. Vel. (m/s):	0.0297	
Schultz Vel. @ Capitol St.:	0.0300	

Table 2.4: 5-Year Flows

Column Number	Grid Cell Width	Flow Velocity
(Row 30)	(meters)	(m/s)
1	45.56	0.600
2	41.37	0.860
3	38.84	0.986
4	36.58	1.024
5	34.5	1.023
6	32.59	0.974
7	30.83	0.853
8	29.24	0.713
9	27.79	0.541
10	25.74	0.231
Sum = 343		
Mass Rate In (cms):	470	
Mass Rate Out (cms):	470	
Width Avg. Vel. (m/s):	0.798	
HEC-RAS Vel. (m/s):	0.990	

Table 2.5: 10-Year Flows

Column Number	Grid Cell Width	Flow Velocity
(Row 30)	(meters)	(m/s)
1	45.56	0.802
2	41.37	1.090
3	38.84	1.248
4	36.58	1.305
5	34.5	1.308
6	32.59	1.248
7	30.83	1.088
8	29.24	0.899
9	27.79	0.682
10	25.74	0.272
Sum = 343		
Mass Rate In (cms):	621	
Mass Rate Out (cms):	621	
Width Avg. Vel. (m/s):	1.019	
HEC-RAS Vel. (m/s):	1.190	

Table 2.6: 25-Year Flows

Column Number	Grid Cell Width	Flow Velocity
(Row 30)	(meters)	(m/s)
1	45.56	1.071
2	41.37	1.394
3	38.84	1.588
4	36.58	1.667
5	34.5	1.677
6	32.59	1.605
7	30.83	1.398
8	29.24	1.147
9	27.79	0.838
10	25.74	0.308
Sum = 343		
Mass Rate In (cms):	827	
Mass Rate Out (cms):	827	
Width Avg. Vel. (m/s):	1.304	
HEC-RAS Vel. (m/s):	1.430	

Table 2.7: 50-Year Flows

Column Number	Grid Cell Width	Flow Velocity
(Row 30)	(meters)	(m/s)
1	45.56	1.282
2	41.37	1.614
3	38.84	1.828
4	36.58	1.921
5	34.50	1.936
6	32.59	1.859
7	30.83	1.621
8	29.24	1.326
9	27.79	0.944
10	25.74	0.330
Sum = 343		
Mass Rate In (cms):	979	
Mass Rate Out (cms):	979	
Width Avg. Vel. (m/s):	1.508	
HEC-RAS Vel. (m/s):	1.570	

Table 2.8: 100-Year Flows

Column Number	Grid Cell Width	Flow Velocity
(Row 30)	(meters)	(m/s)
1	45.56	1.491
2	41.37	1.844
3	38.84	2.073
4	36.58	2.180
5	34.50	2.200
6	32.59	2.118
7	30.83	1.852
8	29.24	1.515
9	27.79	1.023
10	25.74	0.339
	Sum = 343	
Mass Rate In (cms):	1140	
Mass Rate Out (cms):	1140	
Width Avg. Vel. (m/s):	1.714	
HEC-RAS Vel. (m/s):	1.670	

Table 2.9: Flow Velocities for All Flows

Flow Regime	Flow Velocity
	(m/s)
Typical Year	0.0297
5-Year Storm	0.798
10-Year Storm	1.019
25-Year Storm	1.304
50-Year Storm	1.508
100-Year Storm	1.714

A sensitivity analysis of the dimensionless drag coefficient and using varying flow velocities for a typical year revealed that a C_f of 0.0025 (the lowest allowable input value) best represented those conditions present in the Anacostia River. As model projected velocities were below those of field measurements and no reliable field data was available to develop a C_f , it was decided to allow the variable to remain at the default value of 0.0025 in an attempt to increase flow velocities as close to field measured velocities as possible. Analysis of the results of this

analysis confirms that the model is sensitive to C_f inputs at low flow velocities (i.e. $\sim 5 \text{ m}^3/\text{sec}$; this value was used in model simulations for Table 2.3). This analysis can be seen in Figure 2.2.

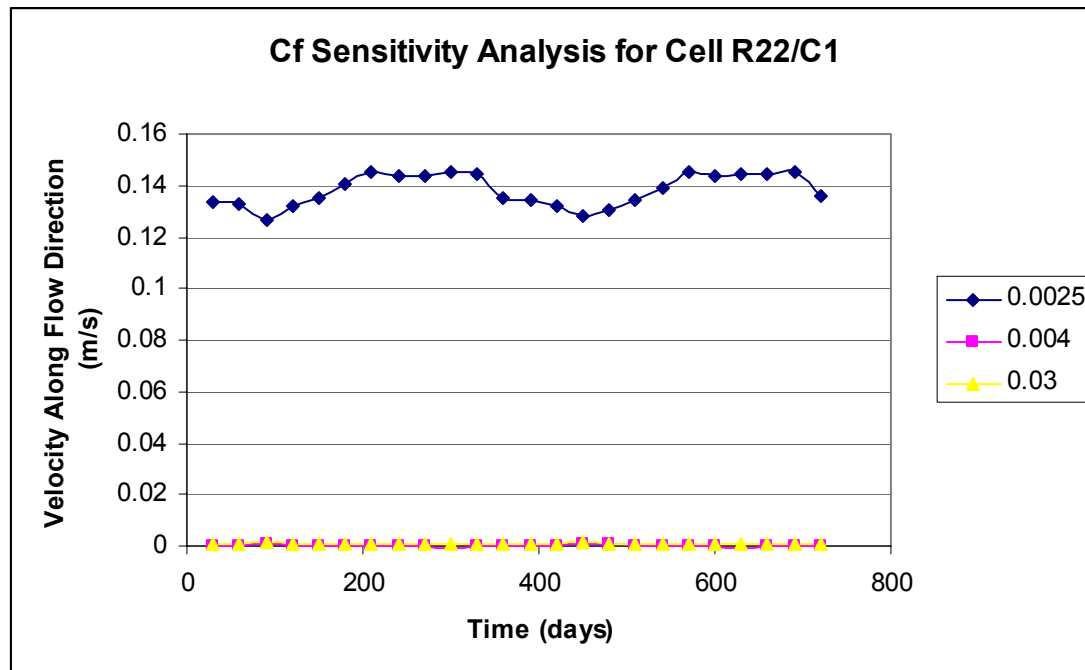


Figure 2.2: C_f Sensitivity

2.5 Conclusions and Recommendations for Future Improvements

2.5.1 Conclusions

Comparisons of MARS-produced flow velocities to those of HEC-RAS model runs indicate that the MARS results are reasonable predictions (within one order of magnitude) of river flow events and those flow velocity discrepancies present (see Table 2.10) are assumed to not drastically affect sediment transport model results, which will be independently verified using field data. Those discrepancies present are assumed to have been a result of the inability to accurately model the tidally influenced hydrodynamics of the Anacostia.

2.5.2 Recommendations for Future Improvements

One area of suggestion for future modifications to the MARS hydrodynamic model would include the addition of user-supplied upstream boundary conditions (i.e., input of tidal

amplitudes at both upstream and downstream boundaries) on tidal simulations. This addition would allow for more accurate representations of the effects of tidal fluctuations throughout the river section being modeled.

Table 2.10: Comparison of Flow Velocities

Width Averaged Downstream Flow Velocities (m/sec) at Capitol Street Bridge						
Flow Event	Normal	5-year	10-year	25-year	50-year	100-year
HEC-RAS (Schultz, 2001 for "Normal")	0.030	0.990	1.190	1.430	1.570	1.670
MARS	0.0297	0.798	1.019	1.304	1.508	1.714
Percent Difference	1.01	21.48	15.48	9.22	4.03	2.60

Chapter 3: Sediment Transport Modeling of the Anacostia River

The sediment transport modeling portion of the MARS is based upon the SEDZL modeling package developed by Zeigler and Lick (Zeigler and Lick, 1986). Prior to the introduction of MARS, HydroQual had combined both the ECOM hydrodynamic model (the precursor to MARS' hydrodynamic model) and the SEDZL sediment transport model into the ECOMSED model. The ECOMSED model employed the composite modeling packages in an effort to produce a comprehensive modeling system capable of accurately representing both river flow characteristics and sediment transport properties and became the foundation for the sediment transport portion of the MARS model.

In order to effectively simulate the migration and transport of chemicals in a natural riverine system, the MARS package was subsequently modified to focus primarily upon the transport of cohesive sediments (e.g. aggregation into flocs, settling properties, self-armoring, etc.), since this class of sediments has the most impact on chemical fate and transport. As a result of this modification, the sediment transport portion of the MARS model does not effectively simulate non-cohesive sediments.

The sediment transport equation used in the MARS model is (Jain, 2003):

$$\frac{\partial DC}{\partial t} + \frac{\partial DV_x C}{\partial x} + \frac{\partial DV_y C}{\partial y} = \frac{\partial}{\partial x} (DA_h \frac{\partial C}{\partial y}) + E_f - D_f \quad (\text{Equation 3-1})$$

Where: D = depth of water column (length)

C = vertically averaged suspended cohesive sediment solids concentration (mass/length³)

t = time

V_x = vertically averaged water current in the x direction (length/time)

V_y = vertically averaged water current in the y direction (length/time)

A_h = horizontal eddy diffusivity (length²/time)

E_f = erosion flux (mass/(length²·time))

D_f = deposition flux (mass/(length²·time))

Assuming all mass conserved and a vertically averaged water column

During model computations, mass balances are conducted on all individual grid cells within the segmentation grid. This ensures mass (sediments) is conserved within the river system as a whole as particles are transported between adjacent grid cells. Using the water flow rates and velocities from the hydrodynamics, the sediment mass balance in MARS is given by (Jain, 2003):

$$V \frac{\partial C}{\partial t} = \sum_{in} QC_c - \sum_{out} QC + \sum E'(C_c - C) + E_f A - D_f A \quad (\text{Equation 3-2})$$

Where: V = volume of cell (length^3)

C = averaged suspended cohesive sediment concentration within cell ($\text{mass}/\text{length}^3$)

t = time

Q = water flow rate ($\text{length}^3/\text{time}$)

C_c = averaged suspended cohesive sediment concentration within connecting cell ($\text{mass}/\text{length}^3$)

E' = bulk dispersion coefficient ($\text{length}^3/\text{time}$)

E_f = erosion flux ($\text{mass}/(\text{length}^2 \cdot \text{time})$)

A = area of sediment-water interface (length^2)

D_f = deposition flux ($\text{mass}/(\text{length}^2 \cdot \text{time})$)

Assuming a vertically averaged water column, eventual self armoring of the sediment bed, and a finite difference solution

3.1 Description of MARS Hydrodynamic Model Variables and Inputs

The MARS modeling package requires the input of 23 user-provided variables and/or constants to simulate the sediment transport properties of a river system. While all inputs are accompanied with default values and limiting ranges of possible values, the accuracy of these inputs is vital to the successful modeling of the sediment bed deposition and/or erosion associated with a given flow event. Due to the varying nature of certain river and flow event characteristics, sensitivity analyses should be conducted on those variables deemed to have the most influence on model outputs. These analyses, along with model results, will be discussed in depth in the Results section of this chapter.

Information regarding representative sediment properties for the demonstration area can be found in Appendix D.

3.1.1 Print Interval

The print interval input is, in basic, the reporting interval for the model. Model results will be displayed for each interval possible given the specified LOS. For instance, a model run with a stipulated LOS of ninety days and a reporting interval of thirty days will allow for three data points to be displayed in the model results (one data point at each the thirty, sixty, and ninety day times). As with the LOS, computational time is directly related to the print interval input selected. It should be noted however, that the model requires that there be at least two full reporting intervals within a given length of simulation. Failure to do so will result in a model error.

The default value for the print interval is set at thirty days and there exists no upper bound on value. The minimum value for print interval is set at 0.041667 days (i.e. one hour) (Jain, 2003).

3.1.2 Dry Density

The dry density input parameter is a constant value used by MARS in the determination of erosional and/or depositional areas. The default value given by the program for this input is 0.87 g/cc and an upper bound is set to 3 g/cc (Jain, 2003). This parameter is best determined from analysis of field samples and care should be taken that a sufficient number of samples be obtained to ensure a statistical representation of the sediments present in the area of interest.

3.1.3 Bottom Friction Coefficient

The bottom friction coefficient (f_w) is a constant input parameter employed by MARS in establishing shear stresses exerted at the sediment-water interface by wind-driven waves. The

model provides a default value of 0.0025 and upper and lower bounds of acceptable input values for the parameter are established at 0.03 and 0.0025, respectively. The equation for determining bottom friction coefficients is (van Rijn, 1983):

$$f_w = \exp \left[-6 + 5.2 \left(\frac{A_p}{k_s} \right)^{-0.19} \right] \quad (\text{Equation 3.1-1})$$

Where: f_w = bottom friction coefficient
 A_p = peak orbital excursion (meter)
 k_s = equivalent/effective bed roughness (meter)

The equation for determining peak orbital excursion is (Jain, 2003):

$$A_p = \frac{H}{2 \sinh \left(\frac{2\pi d}{L} \right)} \quad (\text{Equation 3.1-2})$$

Where: A_p = peak orbital excursion (meter)
 H = significant wave height (meter)
 d = depth of water column (meter)
 L = significant wave length (meter)

The equation for determining significant wave height is (USACOE, 1984):

$$H = \frac{U^2}{g} 0.283 \tanh \left[0.530 \left(\frac{gd}{U^2} \right)^{0.75} \right] \tanh \left[\frac{0.0125 \left(\frac{gF}{U^2} \right)^{0.42}}{\tanh \left[0.530 \left(\frac{gd}{U^2} \right)^{0.75} \right]} \right] \quad (\text{Equation 3.1-3})$$

Where: H = significant wave height (meter)
 U = wind speed (meter/second)
 g = gravitational acceleration = 9.81 (meter/second²)
 d = depth of water column (meter)
 F = fetch length (meter)

The equation for determining significant wave length is (USACOE, 1984):

$$L = T \sqrt{gd} \quad (\text{Equation 3.1-4})$$

Where: L = significant wave length (meter)
 T = significant wave period (second)
 g = gravitational acceleration = 9.81 (meter/second²)

The equation for determining significant wave period is (USACOE, 1984):

$$T = \frac{2U\pi}{g} \tanh \left[0.833 \left(\frac{gd}{U^2} \right)^{0.375} \right] \tanh \left[\frac{0.077 \left(\frac{gF}{U^2} \right)^{0.25}}{\tanh \left[0.833 \left(\frac{gd}{U^2} \right)^{0.375} \right]} \right] \quad (\text{Equation 3.1-5})$$

Where: T = significant wave height (meter)
 U = wind speed (meter/second)
 g = gravitational acceleration = 9.81 (meter/second²)
 d = depth of water column (meter)
 F = fetch length (meter)

The wind-driven wave shear stress is combined with the water current induced shear stress to produce the total shear stress exerted on the sediment bed at the sediment-water interface. The equation for total shear stress is (Jain, 2003):

$$\tau_t = \tau_w + \tau_c \quad (\text{Equation 3.1-6})$$

Where: τ_t = total shear stress (Newton/meter²)
 τ_w = wind-driven wave induced shear stress (Newton/meter²)
 τ_c = water current induced shear stress (Newton/meter²)

Upon model execution, the user-supplied bottom friction coefficient is used to establish shear stress at the sediment-water interface as a result of wind-induced waves. The equation for this shear stress is (Jain, 2003):

$$\tau_w = 0.5 f_w U_p^2 \rho \quad (\text{Equation 3.1-7})$$

Where: τ_w = instantaneous wind-driven wave shear stress (Newton/meter²)
 f_w = bottom friction coefficient
 U_p = peak orbital velocity (meter/second)
 ρ = water density (kilogram/meter³)

The equation used to determine peak orbital velocity is (USACOE, 1984):

$$U_p = \frac{\pi H}{T \sinh\left(\frac{2\pi d}{L}\right)} \quad (\text{Equation 3.1-8})$$

Where: U_p = peak orbital velocity (meter/second)

H = significant wave height (meter)

T = significant wave period (second)

d = depth of water column (meter)

L = significant wave length (meter)

3.1.4 Initial Concentration

The initial concentration parameter is a constant input used by the sediment transport portion of the MARS model to establish an initial total suspended solids concentration (TSS) in the water column. While the TSS loading of the water column will invariably change during the course of model runs that exhibit any erosion and/or deposition, this initial concentration input allows model users to adjust the sediment transport models to accurately reflect observed river conditions. The MARS model establishes a default initial concentration value at 10 mg/L and has no upper or lower constraints on parameter input (Jain, 2003).

3.1.5 Boundary Concentration

The boundary concentration parameter is a constant employed by the sediment transport model portion of the MARS model to establish the downstream TSS concentration in the water column. The default value for the TSS boundary concentration is set at an initial value of 10 mg/L and has no upper or lower bounds limiting input values (Jain, 2003).

3.1.6 α and β in Settling Equation

The above coefficients are used in the determination of the settling velocity for suspended particles using the following equation (Jain, 2003):

$$W_s = \alpha (CG)^\beta \quad (\text{Equation 3.1-9})$$

Where: W_s = settling velocity ($\mu\text{m}/\text{sec}$)

α = experimentally determined coefficient

C = suspended cohesive sediment concentration (mg/L)

G = water column shear stress (dyne/cm^2)

β = experimentally determined coefficient

The alpha and beta parameters in the settling equation are constant inputs required by the model to determine the settling velocity for suspended cohesive sediments and the resulting depositional flux. These two parameters are, in basic, used to specify the degree of salinity and associated viscosity and water density of the water column. An analysis by HydroQual of previous work done on the subject (Burban et al., 1990) reveals the following table of values (Jain, 2003):

Table 3.1: Settling Equation Parameters

Water Salinity	Alpha ($\mu\text{m}/\text{s}$)	Beta
Freshwater	35	0.14
Saltwater	28	0.22

The resultant settling velocity is then employed in the calculation of the depositional flux to the sediment bed using the following equation (Jain, 2003):

$$D_f = PW_s C \quad (\text{Equation 3.1-10})$$

Where: D_f = depositional flux ($\text{mass}/(\text{length}^2 \cdot \text{time})$)

P = probability of deposition

W_s = settling velocity ($\text{length}/\text{time}$)

C = cell averaged TSS concentration ($\text{mass}/\text{length}^3$)

The probability of deposition can be calculated (Partheniades, 1992) by using an experimental approximation of the probability (Jain, 2003):

$$P = \frac{1}{(2\pi)^{0.5}} e^{\frac{-Y^2}{2}} (0.4362z - 0.1202z^2 + 0.9373z^3) \quad (\text{Equation 3.1-11})$$

Where: $z = (1 + 0.3327y)^{-1}$
 $y < 0$, $P(-y) = 1 - P(y)$ when $(0 \leq y < \text{infinity})$

3.1.7 Critical Shear Stress for Erosion

The critical shear stress parameter, τ_o , is a constant input employed by MARS in determining the threshold of incipient motion for modeling the erosion and eventual armoring of cohesive sediments. A default value for this constant is supplied by the model and set at 0.1 dynes/cm². There are no upper or lower bounds in the sediment transport model restraining possible input values (Jain, 2003). These values can be determined experimentally. The critical shear stress parameter is employed in determining potential sediment erosion through the following equation (Gailani et al., 1991):

$$\varepsilon = \frac{a_o}{T_d^m} \left(\frac{\tau_b - \tau_o}{\tau_o} \right)^n \quad (\text{Equation 3.1-12})$$

Where: $\tau_b > \tau_o$

ε = net mass of sediment eroded per unit surface area (mg/cm²)

a_o = sediment erosion function coefficient

T_d = time after deposition (day)

m = sediment erosion function coefficient

τ_b = bed shear stress (dyne/cm²)

τ_o = effective critical bed shear stress (dyne/cm²)

n = sediment erosion function coefficient

3.1.8 a_o , n , and m in Sediment Erosion Equation

a_o , n , and m in the sediment erosion equation (Equation 3.1-12) are system specific inputs that are typically obtained through shaker studies conducted on in-situ or representative sediment samples (Tsai and Lick, 1986). Typical values of a_o range from 0.071 to 5.4, though the model has a default value for this parameter set at 0.071 mg/cm². A default value for n is established at 3 and exhibits a range of “field values” from 1.74 to 3.00. The input parameter m displays experimentally determined values ranging from 0.5 to 2.0 and has an established default value within the model of 0.5 (Jain, 2003).

3.1.9 Upstream Concentration

The upstream concentration parameter is a time variable input used to establish an upstream boundary condition concerning total suspended solids concentration of cohesive sediments. TSS values for this parameter are allowed to vary with time and may be supplied using imported two-column, tab-delimited spreadsheets. Upstream concentration values should be established from field measurements or using model predicted concentrations. The default value for this parameter is 10 mg/L (Jain, 2003).

3.1.10 Critical Shear Stress, Layers 1 through 7

The critical shear stress, τ_o , parameters for layers 1 through 7 are constant input parameters that are used to establish the threshold of erosion for bed sediments. Values for these inputs can be either experimentally determined or projected using analytical solutions. Default values for these inputs are set at 1.0 dynes/cm² (Jain, 2003).

3.1.11 Time Step

The time step input in the sediment transport portion of the MARS model is used in the solution procedure for the finite difference approximation used in the model. Computational time is inversely proportional to the input time step and, as such, the time step can be adjusted to reduce model execution times. MARS documentation states that an initial time step of 20 seconds should be adequate. If this time step renders the model unstable, subsequent simulations should use smaller time steps. Time steps larger than one should result in stable model executions (Jain, 2003).

3.1.12 Wind Speed

Wind speed is a time variable parameter that is employed by MARS to determine wind-induced wave shear stresses. As with all MARS time-dependent variables, this parameter may

be established by using a two-column, tab-delimited spreadsheet imported at the model prompt. Default values for this input are established at 0 m/sec (Jain, 2003).

3.1.13 Wind Direction

Wind direction is a time variable parameter that is employed by MARS to determine wind-induced wave shear stresses. As with all MARS time-dependent variables, this parameter may be established by using a two-column, tab-delimited spreadsheet imported at the model prompt. Default values for this input are established at 0 degrees North and are allowed to vary from 0 to 360°N (Jain, 2003).

3.2 Development of MARS Sediment Transport Model Variables and Inputs to Simulate Anacostia River Sediment Transport Phenomena

The model parameters employed in the sediment transport modeling of the Anacostia River were developed from both historical and field data as well as from literature sources. All parameters were selected on the basis of providing MARS with the most accurate information available to ensure the proper representation of river characteristics and cohesive sediment transport phenomena in all simulations as well preserving the quality of all model predictions. All sediment transport model parameters were selected based upon the premise of ultimately imposing a steady state (SS) Total Suspended Solids (TSS) loading condition for individual flow event scenarios, as accurate data on storm flow associated sediment loadings is non-existent.

3.2.1 Print Interval

The print interval selected for input in all sediment transport executions was 30 days. This value was selected to maintain a consistent reporting interval.

3.2.2 Dry Density

The dry density input parameter for all sediment transport runs was established at 2.59 g/cc. This value was determined through an analysis of numerous, homogenized surficial

sediment samples collected from the Anacostia River capping demonstration area and analyzed by Soil Testing Engineers (STE, 2003).

Sediment samples were collected from throughout the demonstration area using a box corer capable of collecting samples to an approximate depth of 2 feet below the sediment-water interface and an approximate 4 ft² surficial area. A total of 165 gallons of sediment was collected from the demonstration area during this particular sample collection. All 165 gallons were subsequently homogenized using a large capacity cement mixer and 55-gallon drums before being analyzed to determine physical properties. Results of particle size analyses can be found in Figure 1.1-2.

3.2.3 Bottom Friction Coefficient

The bottom friction coefficient for all sediment transport model executions was established at a value of 0.006. Employing van Rijn's equation (section 3.1.3) and assuming f_w cannot exceed a maximum value of 0.3, the van Rijn inputs, k_s and A_p , were developed through the following assumptions:

$$k_s \approx D_b = D_{50} = 0.027mm \text{ (STE, 2003; Wright, 1989)} \quad (\text{Equation 3.2-1})$$

and $H = 0.3m$, $L = 28.9m$, and $d = 1.83m$, as stated in Appendix B of the Revised Basis of Design Document (Horne, 2003).

3.2.4 Initial Concentration

Previous studies on the Anacostia have shown that 12.5 mg/L is a reasonable estimate of typical year TSS loadings (Chadwick, 2000). Adjustments were not made to the 12.5 mg/L figure to account for sediment fractions which may not be cohesive as no reliable data was available to assist in producing a correction factor. Storm regime TSS loadings were established at 64.5 mg/L. Historical data has shown a predicted TSS loading of 80 mg/L in the

demonstration area of the river when under storm-associated flows. However, only approximately 80 percent of the total storm event load is cohesive sediment so appropriate adjustments were made (Schultz, 2001).

3.2.5 Boundary Concentration

All downstream boundary suspended sediment concentrations were established at the same values as the initial water column TSS-cohesives concentrations due to the proximity of the upstream and downstream boundaries to the capping demonstration area. All model predictions show no discernable difference in suspended sediment concentrations over such a short river reach.

3.2.6 α and β in Settling Equation

The alpha and beta input parameters were selected to represent a fresh water river system, as this stretch of the Anacostia is a predominantly non-saline environment. Accordingly, alpha and beta were established at values of 35.0 um/s and 0.14, respectively (Jain, 2003).

3.2.7 Critical Shear Stress

Previous analyses of Anacostia River sediments have indicated a critical shear stress for sediment deposition of 0.02 N/m² (Schultz, 2001). Appropriate unit conversions produced a model parameter input value of 0.199 dynes/cm².

3.2.8 a_o , n , and m in Sediment Erosion Equation

a_o , n , and m were all allowed to remain at their default values for sediment transport model runs. a_o was established at a value of 0.071 mg/cm². n was allowed to remain at a value of 3 based upon previous experimental results from fine grained sediments indicating that 3 is an acceptable value (Ziegler and Nisbet, 1994). m was also allowed to remain at its assigned default value of 0.5. These values were not determined from experimental analysis of Anacostia River

sediments due to the lack of undisturbed, in-situ sediment samples that would be needed to conduct the required investigations.

3.2.9 Upstream Concentration

All upstream boundary suspended sediment concentrations were established at the same values as the initial water column TSS-cohesives concentrations due to the proximity of the upstream and downstream boundaries to the capping demonstration area. All model predictions show no discernable difference in suspended sediment concentrations over such a short river reach.

3.2.10 Critical Shear Stress, Layers 1 through 7

In order to determine the critical shear stress for incipient motion of the unconsolidated cohesive sediments, the following equation was used (Chien and Wan, 1999):

$$\tau_c = \frac{1}{77.5} \left[3.2(\gamma_s - \gamma)D + \left(\frac{\gamma_b}{\gamma_{b0}} \right)^{10} \frac{k}{D} \right] \quad (\text{Equation 3.2-2})$$

Where: $\gamma = 9.81 \text{ kN/m}^3$ (specific weight of water)
 $\gamma_s = 2.59$ (specific weight of sediment)
 $\gamma_{b0} = 1.6$
 $\gamma_b = 1.09$ (unit weight of sediment including porosity factors)
 $k = 2.9 \times 10^{-4} \text{ g/cm}^2$
 $D = D_{50} = 0.027 \text{ mm}$

$$\gamma_b = \gamma_s(1 - n) \quad (\text{Equation 3.2-3})$$

Where: $n = e/(1+e) = 57.9\%$ (Coduto, 1999; Horne, 2003)
 $e = \text{void ratio} = 1.378$ (Horne, 2003)

The critical shear stress for incipient motion of the uppermost layer (unconsolidated) of sediment (layer 1) in the sediment column was determined from the above equation to be 0.205 dynes/cm^2 , similar to results obtained by Schultz, (2001)

Sediment layers below the sediment-water interface, believed to be consolidated, were established using the following equation (Smerdon and Beasley, 1959):

$$\tau_c = 0.017(PI)^{0.84} \quad (\text{Equation 3.2-4})$$

Where: PI = Plasticity Index = 28 for Sample Location B-4 (Horne, 2003)

The resultant shear stress of consolidated layers of the cohesive sediments was determined to be 27.38 dynes/cm². As this value is quite large, simulations were done to test the affect on sediment bed erosion when the entire sediment column is defined as unconsolidated versus sediment bed erosion when the entire sediment column is defined as being consolidated. This analysis will be discussed in the Conclusions section of the chapter.

3.2.11 Time Step

The time step input parameter for all sediment transport runs was set to 10 seconds. This time step resulted in stable simulations and decreased model computational times.

3.2.12 Wind Speed

Input parameters concerning wind speed were developed from 66 years of averaged historical data gathered at Reagan National Airport in Washington, D.C and collected by the National Virtual Data System, a division of the National Oceanographic and Atmospheric Administration (NOAA). Statistical averages on a monthly basis are provided in Table 3.2.

3.2.13 Wind Direction

Input parameters concerning wind direction were developed from 66 years of averaged historical data gathered at Reagan National Airport in Washington, D.C and collected by the National Virtual Data System, a division of the National Oceanographic and Atmospheric Administration (NOAA). Statistical averages on a monthly basis are provided in Table 3.2.

Table 3.2: Historical Wind Data

Washington National Airport													
	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV	DEC	AVG
DIR	NNW	NW	NNW	S	S	S	S	S	S	S	S	NW	S
SPD (MPH)	10	11	11	11	10	9	9	8	9	9	10	10	10
Peak Gust	51	49	55	48	60	59	63	53	54	58	59	56	63

3.3 MARS Sediment Transport Model Results

Sediment transport model results were verified using X-radiographic and ^{210}Pb , ^{137}Cs and ^7Be geochronological analyses of multicores collected from the lower Anacostia River in March 2003 (Chan and Bentley, 2004). This report will be discussed in the Conclusions section of the chapter. Furthermore, all literature reviews of previous Anacostia sedimentation studies indicate that the capping demonstration zone is located in an area of deposition, which was corroborated by MARS sediment transport model results.

3.3.1 Sediment Transport Model Results

Sediment transport runs were conducted in the following manner:

Table 3.3: Sediment Transport Information

Flow Type	Normal	5-year	10-year	25-year	50-year	100-year
Tidal Flow Rate (cms)	65	470	621	827	979	1140
TSS Loading (mg/L)	12.5	64.5	64.5	64.5	64.5	64.5

The model produced sedimentation rate in the demonstration area was approximately 0.40 cm/yr. Sediment bed cores taken from the Anacostia River and analyzed using X-radiographic and ^{210}Pb , ^{137}Cs and ^7Be geochronological analyses (see Appendix B) revealed historic sedimentation rates (found in Table 3.4) relatively consistent with MARS projections. Discrepancies between model projections and field data could be attributed to a lack of accurate daily field measurements of TSS loadings in the Anacostia River near the demonstration area.

Table 3.4: Sediment Core Dating

Station	²¹⁰ Pb Accumulation rate, S (cm/yr)	Correlation Coefficient, r ²	¹³⁷ Cs Accumulation rate, S (cm/yr)	Biodiffusion Coefficient, Db (cm ² /yr)	Correlation Coefficient, r ²
A2-2	0.66	0.84	>0.4	24	0.86
A3-2	1.00	0.48	>0.8	34	0.88
A4-2	0.61	0.79	>0.7	29	0.67

Low-frequency storm event flow conditions yielded only minor erosion of the sediment column, with the upstream grid cell (R21/C1) experiencing more erosion than the downstream cell (R22/C1). This difference was to be expected as grid cell R21/C1 is located nearer an outside bend of the river and, as such, is subject to additional bed stresses exerted by the flow. Erosion of the bed sediments was limited in all cases as cohesive sediment beds have been shown to armor themselves against erosive forces once a finite amount of sediment has been eroded (Tsai and Lick, 1987).

Results for sediment transport models in the capping demonstration area (R21/C1, R22/C1) can be found in Figures 3.1 through 3.6.

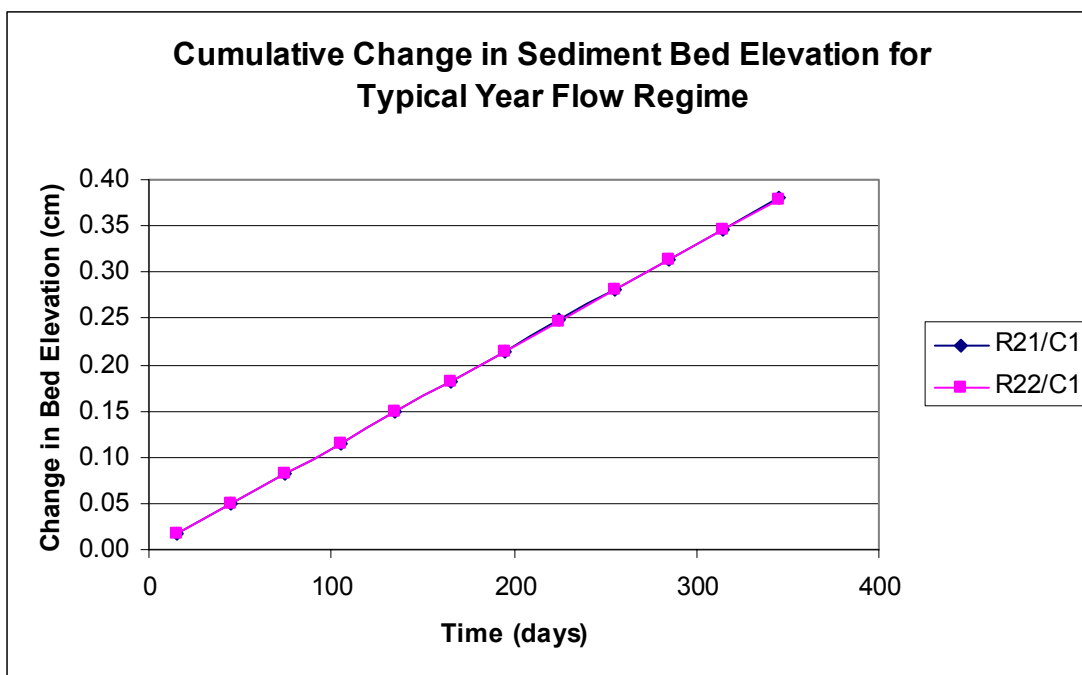


Figure 3.1: Typical Year Bed Elevation

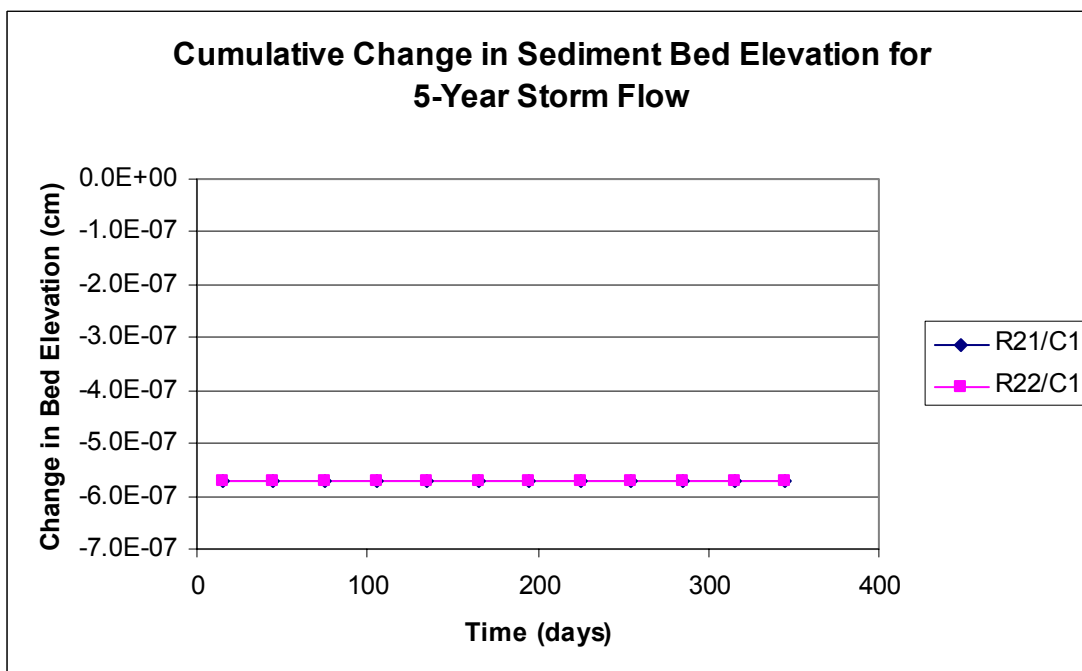


Figure 3.2: 5-Year Flood Bed Elevation

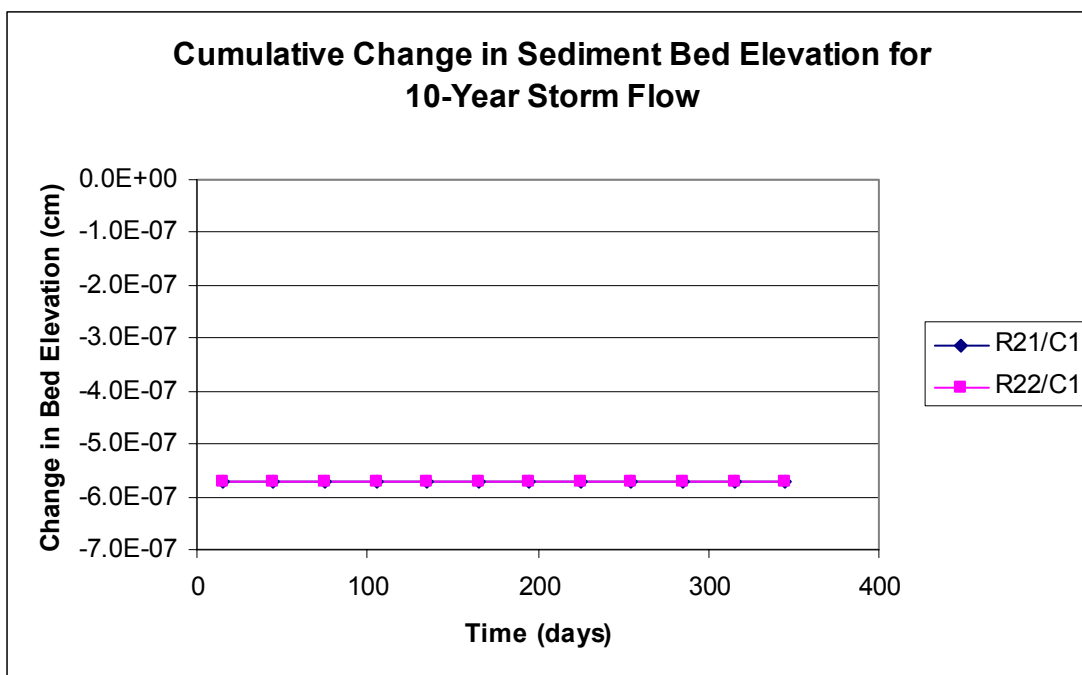


Figure 3.3: 10-Year Flood Bed Elevation

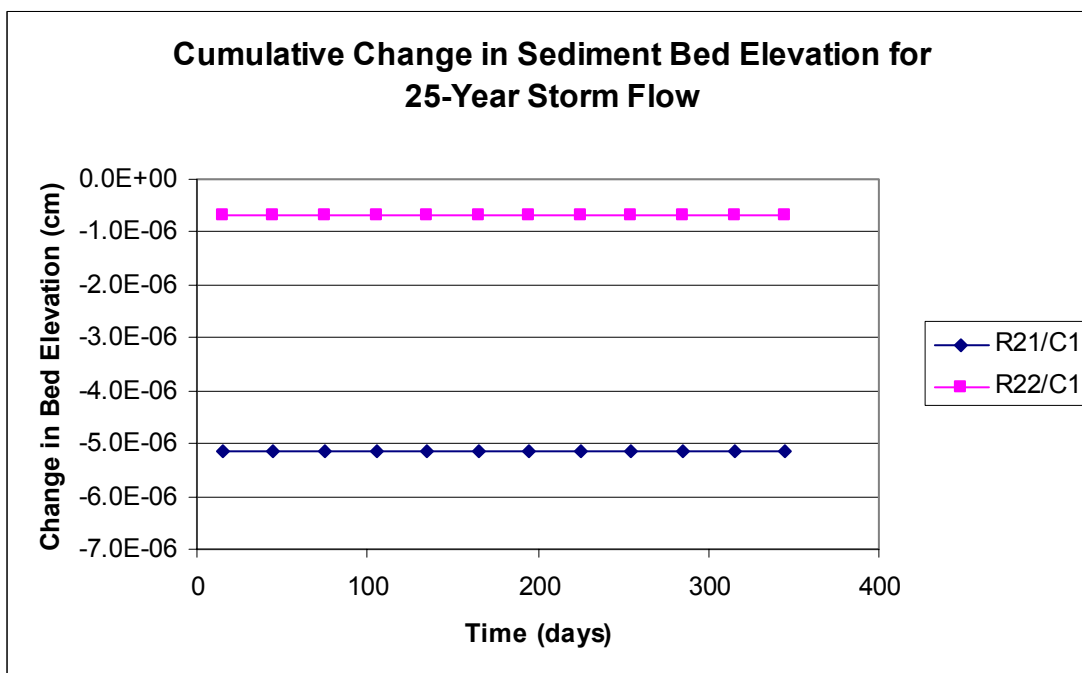


Figure 3.4: 25-Year Flood Bed Elevation

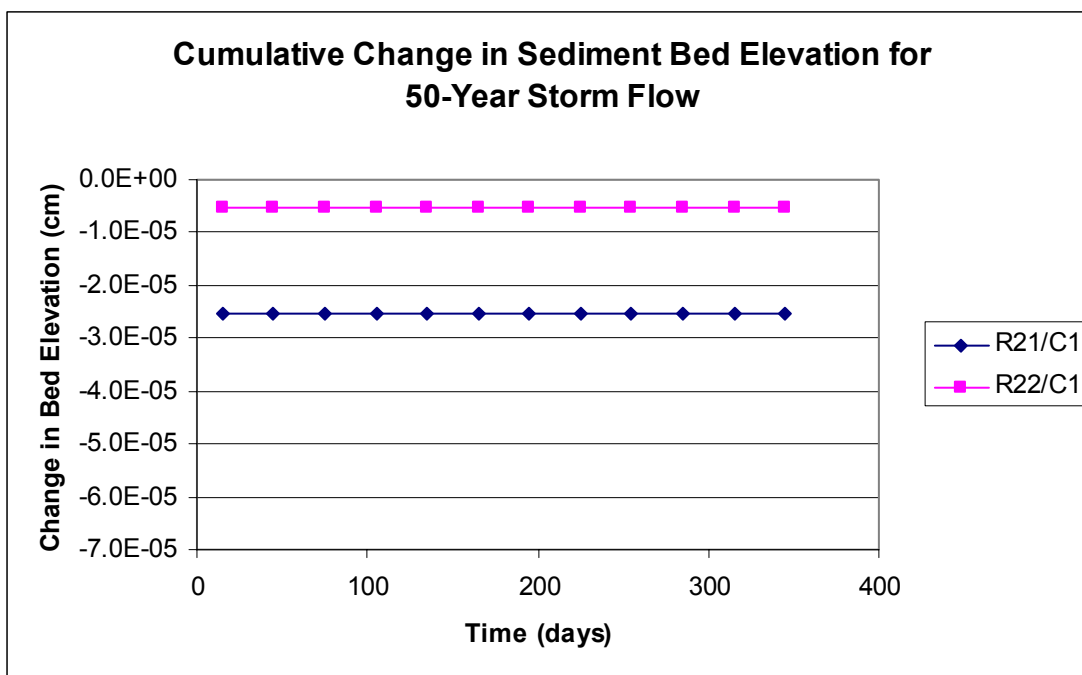


Figure 3.5: 50-Year Flood Bed Elevation

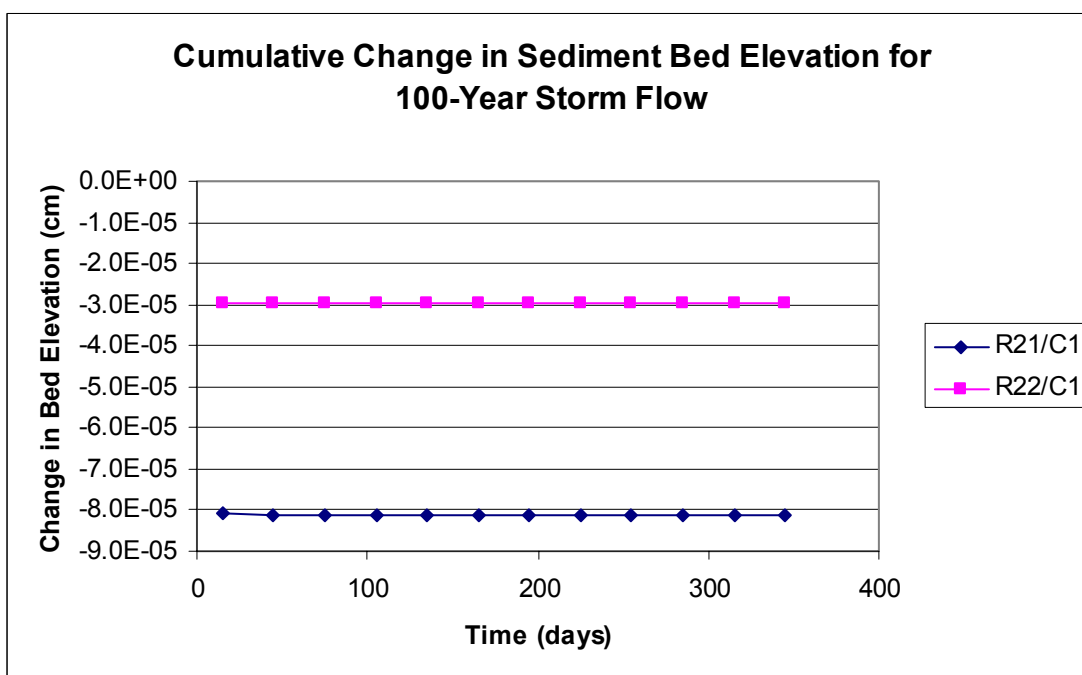


Figure 3.6: 100-Year Flood Bed Elevation

3.4 Conclusions and Recommendations for Future Improvements

3.4.1 Conclusions

Review of the MARS sediment transport model results reveals the demonstration area is a zone of deposition during typical flow regimes. The absence of significant sediment bed erosion during high volume flow events in the capping demonstration area indicates that cap armoring is not required to preserve the geotechnical stability of the reactive barriers, provided that the capping materials have higher critical shear stresses than the sediments.

Analysis of storm event floods reveals that the capping demonstration area, even when subjected to long duration scouring events, does not display exceedingly high rates of sediment bed erosion (See Figures 3.2 through 3.6). Sensitivity analyses were then done to determine if the high critical shear stresses of sediment layers 2-7 (the consolidated layers) had an impact on erosion processes. Model results indicated that there was no additional erosion of sediments (100-year storm) when sediment layers 2-7 were defined as having the same critical shear stress for erosion as the uppermost sediment layer (0.205 dynes/cm^2).

As a result of the above simulations, it is believed that this erosional resistance of the sediment column is a result of channel geometry as the capping demonstration area is situated on the northern most bank of the Anacostia, downstream from an outside bend of the channel. This location reduces the full scouring effects of the channel flow.

3.4.2 Recommendations for Future Improvements

One area which could be considered for future MARS sediment transport model revisions would be the ability of the model to handle non-cohesive sediment transport, which is essential for determining the possible erosion of a sand cap. Such a model capability would allow for the

simulation of all sediment transport phenomena, not just those most often associated with modeling chemical fate and transport.

An additional observation which could be implemented in future model revisions would be the ability to stipulate sediment erosion/deposition characteristics on a spatially variable basis. By allowing all sediment properties (density, shear stresses, etc.) to be stipulated as a spatial variable on the segmentation grid, model users would be able to easily determine the geotechnical stability of capping barriers as well as the general sediment bed. While such a model modification would drastically increase model computation time, it is believed that such a revision could prove to be a powerful tool for future model users.

Chapter 4: Chemical Fate and Transport Modeling in Anacostia River Sediments

The chemical fate and transport portion of the MARS modeling software is a variation of a previous HydroQual chemical transfer model, RCATOX, which in turn was based upon the WASTOX model developed by the USEPA and Manhattan College (Connolly and Winfield, 1984). However, unlike previous versions of RCATOX, the MARS chemical fate and transport modeling packages assumes a vertically homogenous surface water column, thereby diminishing computational time (Jain, 2003).

4.1 Description of MARS Chemical Fate and Transport Model Variables and Inputs

The MARS modeling package requires the input of 70 user-provided variables and/or constants to efficiently simulate the chemical fate and transport phenomena in the Anacostia River sediment columns, caps, and water column. While all inputs are accompanied with default values and limiting ranges of possible values, the accuracy of these inputs is vital to successful modeling of the chemical migration through and out of the sediment bed.

The general governing equation for the chemical fate and transport model is a cell mass balance represented by (Jain, 2003):

$$V \frac{\partial C}{\partial t} = \sum_{IN} Q_C C_C - \sum_{OUT} Q_C C + \sum E' (C_C - C) - KCV \pm SA \quad (\text{Equation 4.1-1})$$

Where: V = volume of cell (length³)

C = cell averaged total chemical concentration (mass/length³)

t = time

Q_C = flow rate (length³/time)

C_C = cell averaged total chemical concentration in connecting cell (mass/length³)

E' = bulk dispersion coefficient (length³/time)

K = kinetic losses (1/time)

S = sediment bed exchange (mass/length²·time)

A = area of water column-sediment bed interface (length²)

4.1.1 Dissolved and DOC Biodegradation Rate Constant at 20°C

The dissolved and DOC biodegradation coefficient at 20°C (K_{bio}) is a constant input parameter which establishes the rate of contaminant degradation by such microorganisms as bacteria and, in limited cases, fungi on dissolved contaminants (Jain, 2003). The parameter is provided with an established default value of 0 L/day-num and is bounded on the lower extreme by 0. There is no established upper bound constraining input values for this parameter. Typical biodegradation rates for select PAH contaminants can be found in Schnoor, 1996 and Chapra, 1997 (Jain, 2003).

The biodegradation equation used in the MARS model is (Jain, 2003):

$$\frac{dC}{dt} = -\frac{V_{max}CB}{k_M} = -K_{BIO}CB \quad (\text{Equation 4.1-2})$$

Where: C = chemical concentration (mass/length³)

t = time

V_{max} = maximum rate of substrate utilization (mass/number·time)

B = bacteria concentration (mass/length³)

k_M = Michaelis half saturation constant (mass/length³); typically 0.1 to 10 mg/L

The bacteria growth rate can be expressed by the equation (Jain, 2003):

$$\frac{dB}{dt} = -a \frac{dC}{dt} \quad (\text{Equation 4.1-3})$$

Where: a = yield coefficient for bacteria utilizing chemical

4.1.2 Dissolved K_{bio} Temperature Correction

The dissolved K_{bio} temperature correction (θ) is a constant input parameter provided by the model to allow for temperature based adjustments to be made to the rate of biodegradation of dissolved contaminants. The default value for this parameter is established at 1.0 and is constrained on the lower and upper bounds by 1.04 and 1.095, respectively (Jain, 2003). To ensure model execution, one must change the correction parameter to an acceptable value.

A typical temperature correction equation is as follows (Jain, 2003):

$$K_{X,T} = K_{X,20^{\circ}C} \theta^{T-20} \quad (\text{Equation 4.1-4})$$

Where: $K_{X,T}$ = degradation rate constant of process X, at temperature T

$K_{X,20^{\circ}C}$ = degradation rate constant of process X, at 20 C

Θ = temperature correction

4.1.3 Sediment Dissolved and DOC Bacteria Density

The sediment dissolved and DOC bacteria density is a constant input parameter employed by the MARS model in establishing the density of those bacteria populations that are neither in the water column nor on the bed solids (i.e., pore water). The model provided default value is 0 num/L, which is also the lower bound. There is no upper bound for this constant input parameter (Jain, 2003).

4.1.4 Sediment Solids Bacteria Density

The sediment solids bacteria density is a constant input parameter used by the MARS model to establish bacteria counts present on sediments. The default value for this parameter is established at 0 num/mg, which is also its lower bound. There exists no upper limit for this input parameter. The typical field value from Chapra, 1997 for bacteria counts on stream sediments is 10^4 - 10^5 num/mg (Jain, 2003).

4.1.5 Solids Biodegradation Rate Constant at 20°C

The solids biodegradation coefficient at 20°C (K_{bio}) is a constant input parameter which establishes the rate of contaminant degradation by such microorganisms as bacteria and, in limited cases, fungi on sorbed contaminants (Jain, 2003). The parameter is provided with an established default value of 0 L/day-num and is bounded on the lower extreme by 0. There is no established upper bound constraining input values for this parameter. Typical biodegradation rates for select PAH contaminants can be found in Schnoor, 1996 and Chapra, 1997 (Jain, 2003).

The biodegradation equation used in the MARS model can be found in section 4.1.1.

4.1.6 Solids K_{bio} Temperature Correction

The solids K_{bio} temperature correction (θ) is a constant input parameter provided by the model to allow for temperature based adjustments to be made to the rate of biodegradation of sorbed contaminants. The default value for this parameter is established at 1.0 and is constrained on the lower and upper bounds by 1.04 and 1.095, respectively (Jain, 2003). To ensure model execution, one must change the correction parameter to an acceptable value.

A typical temperature correction equation can be found in section 4.1.2.

4.1.7 Water Column Dissolved & Dissolved Organic Carbon Bacteria Density

The water column dissolved and DOC bacteria density is a constant input parameter employed by the MARS model in establishing the density of those bacteria populations that are in the water. The model provided default value is 0 num/L and is constrained on the lower bound by 0 as well. There is no upper bound for this constant input parameter. The typical field value from Chapra, 1997 for bacteria counts in surficial waters is 50000 to 1×10^9 num/L (Jain, 2003).

4.1.8 Water Column Solids Bacteria Density

The water column solids bacteria density is a constant input parameter employed by the MARS model in establishing the density of those bacteria populations on suspended solids in the water column. The model provided default value is 0 num/mg and is constrained on the lower bound by 0 as well. There is no upper bound for this constant input parameter (Jain, 2003).

4.1.9 Downstream Boundary Concentration

The downstream boundary concentration is a constant input parameter employed by the MARS model in establishing dissolved contaminant concentrations within the water column at

the defined downstream boundary. The default value for this parameter within the model is 0.0001 mg/L, with no upper bound and a lower bound of 0 mg/L (Jain, 2003).

4.1.10 Upstream Boundary Concentration

The upstream boundary concentration is a constant input parameter employed by the MARS model in establishing dissolved contaminant concentrations within the water column at the defined upstream boundary. The default value for this parameter within the model is 0.0001 mg/L, with no upper bound and a lower bound of 0 mg/L (Jain, 2003).

4.1.11 Water Column Initial Concentration

The water column initial concentration is a constant input parameter employed by the MARS model in establishing dissolved contaminant concentrations within the water column at the time of initial model execution. The default value for this parameter within the model is 0.0001 mg/L, with no upper bound and a lower bound of 0 mg/L (Jain, 2003).

4.1.12 Sediment DOC Koc-Solids Koc Ratio

The sediment DOC-solids organic carbon partitioning coefficient ratio is used by the MARS model to define the ratio of the sediment dissolved organic carbon partitioning coefficient to the solids partitioning coefficient and is used to determine DOC partitioning of the contaminant. The default value for this parameter is 0.01 and displays no upper bound. The parameter is confined on the lower bound by 0.

4.1.13 Sediment Bed DOC Concentration

The sediment bed dissolved organic carbon concentration is a constant input parameter employed by the MARS in determining DOC partitioning of the contaminant. Default values for this parameter are established by the model at 25 mg/L. There exists only a lower bound of 0 mg/L for this variable (Jain, 2003).

4.1.14 Water Column DOC Concentration

The water column dissolved organic carbon concentration is a constant input parameter employed by the MARS in determining DOC partitioning of the contaminant. Default values for this parameter are established by the model at 25 mg/L. There exists only a lower bound of 0 mg/L for this variable (Jain, 2003).

4.1.15 Water Column DOC Koc-Solids Koc Ratio

The water column DOC-solids organic carbon partitioning coefficient ratio is used by the MARS model to define the ratio of the water column dissolved organic carbon partitioning coefficient to the solids partitioning coefficient and is used to determine DOC partitioning of the contaminant. The default value for this parameter is 0.01 and displays no upper bound. The parameter is confined on the lower bound by 0.

4.1.16 Chemical Name

The chemical name input parameter is a constant parameter determined by the user's selection from the model-provided chemical wizard whenever a new chemical fate and transport model run is initiated. The wizard, upon selection of a chemical, also establishes the chemical's associated Henry's law constant (H), molecular weight, and log octanol-water partition coefficient (Kow). While the MARS model chemical wizard is currently limited to known PAHs, it does allow for the creation of a chemical (i.e., a PCB) by inputting the associated molecular weight, H, and log Kow values (Jain, 2003).

4.1.17 Print Interval

Basically, the print interval input is the reporting interval for the model. Model results will be displayed for each interval possible given the specified LOS. For instance, a model run with a stipulated LOS of ninety days and a reporting interval of thirty days will allow for three

data points to be displayed in the model results (one data point at each the thirty, sixty, and ninety day times). It should be noted however, that the model requires that there be at least two full reporting intervals within a given length of simulation. Failure to do so will result in a computational model error.

The default value for the print interval is set at thirty days and there exists no upper bound on value. The minimum value for print interval is set at 1 day (Jain, 2003).

4.1.18 Sediment Bed Temperature

The sediment bed temperature is a constant input parameter used by the MARS model in adjusting all temperature dependent chemical transport phenomena, especially biodegradation, volatilization, and hydrolysis. The default value for this parameter is 20.0°C and there exists no lower or upper bounds (Jain, 2003).

It should be noted that extreme values tended to result in model execution complications during experimentation.

4.1.19 Water Column Temperature

The water column temperature is a constant input parameter used by the MARS model in adjusting all temperature dependent chemical transport phenomena, especially biodegradation, volatilization, and hydrolysis. The default value for this parameter is 20.0°C and there exists no lower or upper bounds (Jain, 2003).

It should be noted that extreme values tended to result in model execution complications during experimentation.

4.1.20 Acid Hydrolysis Rate Constant at 20°C

The acid hydrolysis rate constant is a constant input parameter used, along with various other hydrolysis parameters, to determine overall hydrolysis. Both the default and lower bounds

for this parameter are 0 L/mol-day and there exists no upper constraint on input (Jain, 2003).

The hydrolysis equation employed in the MARS model is (Jain, 2003):

$$\frac{dC_d}{dt} = -K_H C_d \quad (\text{Equation 4.1-5})$$

Where: C_d = dissolved concentration (mg/L)

t = time

K_H = overall hydrolysis rate (1/day)

The overall hydrolysis rate can be expressed as (Jain, 2003):

$$K_H = K_n + K_a [H^+] + K_b [OH^-] \quad (\text{Equation 4.1-6})$$

Where: K_H = overall hydrolysis rate (1/day)

K_n = neutral hydrolysis rate constant (1/day)

K_a = acid catalyzed hydrolysis rate constant (1/day)

H^+ = hydrogen ion concentration (mole/L)

OH^- = hydroxide ion concentration (mole/L)

4.1.21 Alkaline Hydrolysis Rate Constant at 20°C

The alkaline hydrolysis rate constant is a constant input parameter used, along with various other hydrolysis parameters, to determine overall hydrolysis. Both the default and lower bounds for this parameter are 0 L/mol-day and there exists no upper constraint on input (Jain, 2003).

The hydrolysis equation employed in the MARS model can be found in section 4.1.19.

4.1.22 Hydrolysis Rate Constant Temperature Correction

The K_H temperature correction (θ) is a constant input parameter provided by the model to allow for temperature based adjustments to be made to the rate of hydrolysis. The default value for this parameter is established at 1.096 and is constrained on the lower bound only by 0 (Jain, 2003).

A typical temperature correction equation can be found in section 4.1.2.

4.1.23 Neutral Hydrolysis Rate Constant at 20°C

The neutral hydrolysis rate constant is a constant input parameter used, along with various other hydrolysis parameters, to determine overall hydrolysis. Both the default and lower bounds for this parameter are 0 L/mol-day and there exists no upper constraint on input (Jain, 2003).

The hydrolysis equation employed in the MARS model can be found in section 4.1.19.

4.1.24 Sediment Bed pH

Sediment bed pH is a constant input parameter employed by the MARS model in further determining the rate of the hydrolysis reaction. The default value for this input is 7.0 and there exist respective upper and lower constraints of 14.0 and 0.0 (Jain, 2003).

4.1.25 Water Column pH

Water column pH is a constant input parameter employed by the MARS model in further determining the rate of the hydrolysis reaction. The default value for this input is 7.0 and there exist respective upper and lower constraints of 14.0 and 0.0 (Jain, 2003).

4.1.26 Sediment Layer Depth

The sediment layer depth parameters are constant inputs used by the model in establishing the depth of the three respective sediment column layers. Layers 1, 2, and 3 (the uppermost, median, and bottom layers, respectively) have defined default values of 5, 10, and 20 cm, respectively. All three layers are confined by a lower bound on input values of 1 cm and exhibit no upper bound (Jain, 2003).

4.1.27 Solids Density

The solids density is a constant input parameter employed by MARS in determining the physical properties of the sediment of interest. A default value of 2.65 g/cc is provided by the

model and there exists no constraints on the bounds of acceptable values for input (Jain, 2003).

4.1.28 Kow-Koc Intercept and Slope

Kow-Koc intercept and slope refer to the y-intercept and slope values of the equation of a line which relates log Kow to log Koc. Due to the fact that the model provides values for log Kow's upon selection of a chemical from the chemical wizard, these two parameters are used solely to determine the value of log Koc. Default values for their input are 1.0 and are limited on the lower bound (due to the log scale) by 0.

The equation used to determine log Koc is as follows:

$$\log K_{oc} = (m)\log K_{ow} + b \quad (\text{Equation 4.1-7})$$

4.1.29 log Kow

Log Kow is a constant input parameter provided by the model upon selection of a chemical from the chemical wizard (or input upon creation of a chemical) and varies depending upon the properties of the individual contaminant. The octanol-water partition coefficient is used in determining solids partitioning (Jain, 2003).

4.1.30 Sediment Bed Fraction Organic Carbon

Sediment bed fraction organic carbon is a constant input parameter employed by the MARS model in determining the overall solids partitioning coefficient. Default values for this parameter are 0.010 and upper and lower bounds for input exist at 0.1 and 0.001, respectively (Jain, 2003).

The equation for determining overall solids partitioning is (Jain, 2003):

$$K_p = foc \cdot K_{oc} \quad (\text{Equation 4.1-8})$$

Where: K_p = overall solids partition coefficient

foc = fraction organic carbon

K_{oc} = organic carbon partitioning coefficient (length³/mass)

4.1.31 Solids Dependent Partition Parameter

The solids dependent partition parameter is a constant input with a model-provided default value of 1.4 and a lower bound of 0.0. The parameter has been shown, through experimentation, to control dissolved and particulate portions of a chemical in a water column (Jain, 2003):

The particle interaction equation is (Jain, 2003):

$$K_p = \frac{K_{p,o}}{1 + \frac{K_{p,o} \cdot m}{v_x}} \quad (\text{Equation 4.1-9})$$

Where: K_p = partitioning coefficient

$K_{p,o}$ = limiting partition coefficient with no particle interaction ($\text{length}^3/\text{mass}$)

m = solids concentration ($\text{mass}/\text{length}^3$)

v_x = ratio of adsorption to particle induced desorption rate, typically on order of 1

4.1.32 Water Column Fraction Organic Carbon

Water column fraction organic carbon is a constant input parameter employed by the MARS model in determining the overall solids partitioning coefficient. Default values for this parameter are 0.010 and upper and lower bounds for input exist at 0.4 and 0.001, respectively (Jain, 2003).

The equation for determining overall solids partitioning can be found in section 4.1.27.

4.1.33 Chemical Molecular Weight

Chemical molecular weight is a compound-specific constant parameter which is provided by the model upon selection of a chemical from the chemical wizard and is used for determining the mass flux of volatilized chemical. Molecular weight can also be input for created contaminants. A default value of 257.55 g/mole is provided for unknown molecular weights (Jain, 2003).

4.1.34 Henry's Law Constant

Henry's law constant is a compound-specific constant parameter which is provided by the model upon selection of a chemical from the chemical wizard and is used for determining the mass flux of volatilized chemical. Henry's law constant can also be input for created contaminants. A default value of 30.0 Pa-m³/mol is provided for unknown Henry's constants (Jain, 2003).

Determination of the gas chemical concentration at the air-water interface is calculated by (Jain, 2003):

$$C_{gi} = H \cdot C_{li} \quad (\text{Equation 4.1-10})$$

Where: C_{gi} = gas chemical concentration at the air-water interface (mass/length³)
H = dimensionless Henry's law constant
 C_{li} = liquid chemical concentration at the air-water interface (mass/length³)

Under steady state conditions, the mass transfer equation at the air-water interface then becomes (Jain, 2003):

$$j = K_L [C_{li} - C_l] = K_G [C_g - C_{gi}] \quad (\text{Equation 4.1-11})$$

Where: j = volatilization mass flux (mass/length²·time)
 K_L = liquid film mass transfer coefficient (length/time)
 C_{li} = liquid chemical concentration at the air-water interface (mass/length³)
 C_l = liquid chemical concentration in bulk liquid (mass/length³)
 K_G = gas film mass transfer coefficient (length/time)
 C_g = gas chemical concentration in bulk gas (mass/length³)
 C_{gi} = gas chemical concentration at air-water interface (mass/length³)

4.1.35 Volatilization Option

The volatilization option is a constant input parameter by which the model user can decide to model chemical volatilization or not. The option is enabled by default (represented by a value of 3) and can be disabled by changing the option value to 0 (Jain, 2003).

4.1.36 Bed Boundary Condition Scale Factor

The bed boundary condition scale factor is a spatially variable input parameter that is employed in establishing the chemical concentration on the sediments at the deepest portions of the sediment column. By establishing a value with the scale factor parameter, a user is able to create a steady state condition of constant chemical concentration at the bottom of the sediment column. This steady state condition can also be a spatially-varying condition. This concentration can be adjusted to represent a time varying chemical concentration by providing input values for the bed boundary condition time series number input as well as for the scale factor (Jain, 2003).

The bed boundary condition scale factor is provided with a default value of 0 mg/kg and can be adjusted to simulate any contaminant loading scenario (Jain, 2003).

4.1.37 Bed Boundary Condition Time Series Number

The bed boundary condition (BC) time series number is a spatial input parameter by which users can vary a grid cell's chemical loading boundary condition on a temporal basis. By indicating explicitly which time series is to be executed, users are able to vary the bed boundary condition by any one of ten user provided possible boundary condition time-varying scenarios. Some example scenarios are displayed in Table 4.1. The default value for this parameter is 0, or a steady state condition (Jain, 2003).

4.1.38 Groundwater Flow Scale Factor

The groundwater flow scale factor is a spatially variable input parameter that is employed in establishing the advective flow of groundwater throughout the sediment column. By establishing a value with the scale factor parameter, a user is able to create a steady state groundwater flow condition. This condition can be adjusted to represent a time varying scenario

Table 4.1: BC/GW Flow Relationships

Desired Value	Scale Factor	Time Series Number	Time Series Value
Zero	0.0	0	--
Constant	value	0	--
Time-Variable	scale	number	scaled value

Taken verbatim from MARS manual (Jain, 2003)

by providing input values for the groundwater flow time series number input as well as for the scale factor (Jain, 2003). Groundwater flow can also vary concurrently on a spatial basis.

The groundwater flow scale factor is provided with a default value of 0 m³/day and can be adjusted to simulate any flow conditions (Jain, 2003).

4.1.39 Groundwater Flow Time Series Number

The groundwater flow time series number is a spatial input parameter by which users can vary a grid cell's groundwater flow on a temporal basis. By indicating explicitly which time series is to be executed, users are able to vary the groundwater flow by any one of ten user-provided possible time-varying flow scenarios. The default value for this parameter is 0, or a steady state condition (Jain, 2003).

4.1.40 Initial Concentrations in Sediment Layers

The initial concentration parameter for sediment layers 1, 2, and 3 is a spatially varying input by which the initial chemical loading concentration on the sediment can be established. This parameter can be varied on a grid cell basis and is provided with a model default value of 0 mg/kg for all sediment layers (Jain, 2003).

4.1.41 Sediment Layer Diffusion Coefficients

The sediment layer diffusion coefficients are spatial variables and can be established for the interfaces between layers 1 and 2, 2 and 3, and 3 and deep (boundary). Default values for all

diffusion coefficients within the sediment column are established at 0.00001 m²/day. To eliminate diffusive transfer of contaminants, this variable can be set to 0.0 m²/day (Jain, 2003).

The governing equation for sediment layer-sediment layer chemical flux is (Jain, 2003):

$$\frac{\partial C}{\partial t} + \frac{\partial V_z C}{\partial z} = \frac{\partial}{\partial z} \left(E_{SED-DIF} \frac{\partial C}{\partial z} \right) - KC \quad (\text{Equation 4.1-12})$$

Where: C = averaged total chemical concentration (mass/length³)

t = time

V_z = groundwater flow velocity in z-direction (length/time)

z = distance in z-direction (length)

E_{SED-DIF} = diffusion coefficient between sediment layers (length²/time)

K = kinetic losses (1/time)

4.1.42 Water Column-Sediment Interface Diffusion Coefficient

The water column-sediment interface diffusion coefficient is a spatial variable employed by the model in determining the diffusion coefficient at the uppermost boundary of the sediment column. As this area of the sediment column is particularly prone to bioturbation and is more suited for chemical transport than the underlying sediment layers, the model defined default value for this parameter is 0.0001 m²/day (Jain, 2003).

The governing equation for chemical diffusion at the sediment-water interface is (Jain, 2003):

$$S_{DIF} = \frac{E_{WC-DIF}}{L} (C_{d, sed} - C_{d, wc}) \quad (\text{Equation 4.1-13})$$

Where: S_{DIF} = chemical mass flux due to diffusion (mass/length²·time)

E_{WC-DIF} = water column-sediment bed diffusion coefficient (length/time²)

L = mixing length (length)

C_{d, sed} = dissolved chemical concentration in sediment bed (mass/length³)

C_{d, wc} = dissolved chemical concentration in water column (mass/length³)

4.1.43 Sediment Bed Solids Concentration

The sediment bed solids concentration is a spatially varying input parameter with a model defined default value of 1.0 kg/L. The solids concentration plays a role in solids partitioning of

the contaminant of interest and can be calculated using the following equation (Jain, 2003):

$$m = (1 - n)\rho_s \quad (\text{Equation 4.1-14})$$

Where: m = solids concentration (mass/length³)

n = porosity

ρ_s = solids density (solids mass/solids volume) (mass/length³)

4.1.44 Bed Boundary Condition Time Series Numbers 1-10

The bed boundary condition time series numbers 1 through 10 are time varying inputs which are employed by the model in varying the chemical concentration at the bottom of the sediment column on a time varying basis. Ten individual scenarios can be established using each of the available inputs which can then be selected using the spatial variable input, “bed boundary condition time series number,” for each grid cell of interest. Default values for these parameters are set at 0 (steady state) but can be adjusted as necessary (Jain, 2003).

4.1.45 Groundwater Flow Time Series Numbers 1-10

The groundwater flow time series numbers 1 through 10 are time varying inputs which are employed by the model in varying the groundwater flow throughout the sediment column. Ten individual scenarios can be established using each of the available inputs which can then be selected using the spatial variable input, “groundwater flow time series number,” for each grid cell of interest. Default values for these parameters are set at 0 (steady state) but can be adjusted as necessary (Jain, 2003).

4.2 Development of MARS Chemical Fate and Transport Model Variables and Inputs to Simulate Contaminant Transport Phenomena

The model parameters employed in the chemical fate and transport modeling of the Anacostia River were developed from both historical and field data as well as from literature and governmental sources on the subject. All parameters were selected on the basis of providing MARS with the most accurate information available to ensure the proper representation of river

characteristics and contaminant transport phenomena in all simulations, as well preserving the quality of all model predictions. All chemical fate and transport model parameters were selected based upon the premise of ultimately imposing a steady state (SS), accurate representation of the chemodynamic environment found in the Anacostia sediments.

4.2.1 Dissolved and DOC Biodegradation Rate Constant at 20°C

The dissolved and DOC biodegradation rate constant was set to a value of 0 for all chemical fate and transport runs. This value was established in an attempt to provide a worst case scenario of contaminant migration by limiting the degree to which the chemical would be broken down before reaching the sediment water interface.

4.2.2 Dissolved K_{bio} Temperature Correction

The dissolved K_{bio} temperature correction input parameter was set to a value of 0 for all chemical fate and transport runs. This value was established due the lack of need to simulate biodegradation of the contaminant of interest. As the rate constant had previously been set to 0, the temperature correction could have feasibly been allowed to remain at its default value setting with no resulting difference in model calculations.

4.2.3 Sediment Dissolved and DOC Bacteria Density

The sediment dissolved and DOC bacteria density input parameter was set at a value of 0 to simulate the absence of biodegrading microorganisms in the sediment column.

4.2.4 Sediment Solids Bacteria Density

The sediment solids bacteria density input parameter was set to a value of 0 to simulate the absence of biodegrading microorganisms in the sediment column.

4.2.5 Solids Biodegradation Rate Constant at 20°C

The solids biodegradation rate constant input parameter was set to a value of 0.

4.2.6 Solids K_{bio} Temperature Correction

The solids K_{bio} temperature correction input parameter was set to a value of 0 to simulate the absence of biodegrading microorganisms in the sediment column.

4.2.7 Water Column Dissolved & Dissolved Organic Carbon Bacteria Density

The water column dissolved and dissolved organic carbon bacteria density input was set to a value of 0 to simulate the absence of biodegrading microorganisms in the water column.

4.2.8 Water Column Solids Bacteria Density

The water column solids bacteria density input parameter was set to a value of 0 to simulate the absence of biodegrading microorganisms in the water column.

4.2.9 Downstream Boundary Concentration

The downstream boundary concentration was allowed to remain at its default value of 0.0001 mg/L for all contaminants as the river water column, for modeling purposes, was assumed to be devoid of chemicals. While actual water-side concentrations of pollutants are fairly low in the Anacostia, it was expected that the contaminant flux (or migration) from the two grid cells of interest in the model would have little to no overall affect on water column concentrations and, as such, the downstream boundary concentrations for all contaminants could be legitimately set to 0.

4.2.10 Upstream Boundary Concentration

The upstream boundary concentrations for all chemical fate and transport runs were set to 0.0001 mg/L as the water column was assumed to be essentially devoid of contaminants.

4.2.11 Water Column Initial Concentration

The water column initial concentrations for all chemical fate and transport runs were set to 0.0001 mg/L as the water column was assumed to be essentially devoid of contaminants.

4.2.12 Sediment DOC Koc-Solids Koc Ratio

The sediment DOC Koc-solids Koc ratio was established at 0.01 for all chemical fate and model runs. This value was chosen due to the fact that dissolved organic carbon and its partitioning qualities were of little to no concern in this particular modeling effort.

4.2.13 Sediment Bed DOC Concentration

Sediment bed DOC concentrations were set to 25 mg/L for all chemical fate and transport model runs.

4.2.14 Water Column DOC Concentration

Water column DOC concentrations were set to 25 mg/L for all chemical fate and transport model runs.

4.2.15 Water Column DOC Koc-Solids Koc Ratio

The water column DOC Koc-solids Koc ratio was established at 0.01 for all model runs.

4.2.16 Chemical Name

The chemical name input parameter for PAHs of interest were chosen from the chemical wizard library during the time of model initialization. The PAH of particular interest to this modeling effort was phenanthrene, as it has historically been one of the more prevalent PAH contaminants in Anacostia River Sediment and, due to its sorption properties, allowed for the most rapid model simulations.

4.2.17 Print Interval

A print interval of thirty days was chosen for all chemical fate and transport model simulations.

4.2.18 Sediment Bed Temperature

Sediment bed temperatures were established at the default value of 20°C.

4.2.19 Water Column Temperature

Sediment bed temperatures were established at the default value of 20°C due to the fact that biodegradation, hydrolysis, and chemical volatile flux at the air-water interface were of little concern to this modeling effort.

4.2.20 Acid Hydrolysis Rate Constant at 20°C

The acid hydrolysis rate constant was established at a value of 0 for all chemical fate and transport model runs. As a result of hydrolysis not being a focus of this study, all hydrolysis associated variables were rendered non-existent so as to prevent their influence on chemical transport phenomena in model executions.

4.2.21 Alkaline Hydrolysis Rate Constant at 20°C

The alkaline hydrolysis rate constant was established at a value of 0 for all chemical fate and transport runs as hydrolysis was of little concern to this particular modeling effort.

4.2.22 Hydrolysis Rate Constant Temperature Correction

The hydrolysis rate constant temperature correction was established at a value of 0 for all chemical fate and transport runs as hydrolysis was of little concern to this particular modeling effort.

4.2.23 Neutral Hydrolysis Rate Constant at 20°C

The neutral hydrolysis rate constant was established at a value of 0 for all chemical fate and transport runs as hydrolysis was of little concern to this particular modeling effort.

4.2.24 Sediment Bed pH

Sediment bed pH values were allowed to remain at the default value of 7 for all model executions as hydrolysis was of little concern to this particular modeling effort.

4.2.25 Water Column pH

Water column pH values were allowed to remain at the default value of 7 for all model executions as hydrolysis was of little concern to this particular modeling effort.

4.2.26 Sediment Layer Depth

Sediment layer depths were as follows in Table 4.2, as indicated by HSRC capping plans (HSRC, 2004):

Table 4.2: Sediment Layer Information

Model Scenario:	Uncapped	Sand	Apatite	Aquablok	Coke Breeze
Layer Number	Depth in centimeters below Sediment-Water Interface				
1	10	30 (cap)	15 (sand cap)	15 (sand cap)	15 (sand cap)
2	10	15	15 (apatite)	15 (Aquablok)	15 (coke breeze)
3	20	20	20	20	20

Note: Those regions highlighted in gray indicate position of underlying sediment

4.2.27 Solids Density

The solids densities for all materials involved in modeling are as follows in Table 4.3:

Table 4.3: Material Density

Material	River Sediment	Sand	Aquablok	Apatite	Coke Breeze
Density (g/cc)	2.59 (STE, 2003)	2.62 (Horne, 2004)	2.65 (Reible, 2004)	1.3 (Cranell, 2004)	0.76 (Lowry, 2004)

4.2.28 Kow-Koc Intercept and Slope

The Kow-Koc intercept and slope were determined based on the following relationships (Di Toro and McGrath, 2000):

$$PAHs \rightarrow \log Koc = 0.00028 + 0.983 \log Kow \quad (\text{Equation 4.2-1})$$

Log Kow-Koc slope and intercept values were used internally by the model to compute log Koc.

4.2.29 log Kow

The log Kow input parameter is provided by the model upon the selection of a contaminant from the chemical wizard. Upon creating a chemical, users must assign a value for log Kow.

4.2.30 Sediment Bed Fraction Organic Carbon

The sediment bed fraction organic carbon (foc) was varied to represent the appropriate value based on the sediment or capping layer it represented. As foc serves a means of controlling contaminant migration, it was adjusted where appropriate to represent the partitioning qualities of certain capping barriers. The input values can be seen in Table 4.4.

4.2.31 Solids Dependent Partition Parameter

The solids dependent partition parameter was assigned a default value of 1.4 for all chemical fate and transport runs. This value was chosen based on a MARS handbook recommendation (Jain, 2003).

Table 4.4: Fraction Organic Carbon Inputs

Material:	Apatite	Aquablok	Coke Breeze	Sand	Sediment
FOC:	0.001	0.001	1.72	0.001	0.07
Source:	Reible, 2004	Reible, 2004	Lowry, 2004	Reible, 2004	Horne, 2003

4.2.32 Water Column Fraction Organic Carbon

The water column fraction organic carbon input parameter was established at 0.07 upon recommendation from committee members due to the fraction organic carbon present in the sediment column (Reible, 2004).

4.2.33 Chemical Molecular Weight

Chemical molecular weights were input into the model by MARS upon selection of a chemical from the chemical wizard. For PCB transport runs, appropriate molecular weights were input by the user through the chemical wizard.

4.2.34 Henry's Law Constant

Henry's law constants were input into the model by MARS upon selection of a chemical from the chemical wizard. For PCB transport runs, the volatilization portion of the model was turned off as relevant Henry's law information was not available.

4.2.35 Volatilization Option

The volatilization option was set to zero ("off") for all model runs as chemical transport at the air-water interface was not of concern and H values were not available for phenanthrene.

4.2.36 Bed Boundary Condition Scale Factor

The bed boundary condition scale factors were established at the following values in Table 4.5 for cells R21/C1 and R22/C1 after determining maximum chemical concentrations in various sediment samples (Horne, 2004):

Table 4.5: Input Chemical Concentrations

Contaminant	Benzo (a) pyrene	Phenanthrene	Pyrene	Bz# 8	Bz# 31	Bz# 70
Concentration (ug/kg)	4700	16000	13000	100	310	180

Total sample concentrations may be viewed in Appendix C.

4.2.37 Bed Boundary Condition Time Series Number

The bed boundary condition time series number was set at 0 (i.e. steady state).

4.2.38 Groundwater Flow Scale Factor

The bed boundary condition scale factors were established at 163 m³/day for grid cell R21/C1 and 187 m³/day for grid cell R22/C1 for all model runs projecting cap efficiency. These

values were determined by multiplying the maximum recorded seepage velocity in the demonstration area (5.5 cm/day) times the respective areas of the individual grid cells (Horne, 2004). Model simulations projecting the effectiveness of Aquablok, however, were provided with adjusted groundwater flow scale factors of 0.163 m³/day and 0.187 m³/day for cells R21/C1 and R22/C1, respectively. This reduction in flow was based upon the difference in hydraulic conductivities between clays and silty materials ((Freeze and Cherry, 1979).

4.2.39 Groundwater Flow Time Series Number

The groundwater flow time series number for all model runs was set to 0 as all executions were modeled as steady state scenarios.

4.2.40 Initial Concentrations in Sediment Layers

The initial concentrations in the various sediment layers were established at either the concentrations in Table 4.5 or 0.0 mg/kg, depending upon the scenario.

4.2.41 Sediment Layer Diffusion Coefficients

Sediment layer diffusion coefficients were established at 0.00001 m²/day based upon literature values for similar scenarios (Thibodeaux, 1996).

4.2.42 Water Column-Sediment Interface Diffusion Coefficient

The water column-sediment interface diffusion coefficient was established at 0.0003 m²/day to simulate a bioturbation driven diffusion zone in the upper sediment column (Chien et al., 2002).

4.2.43 Sediment Bed Solids Concentration

The sediment bed solids concentration was set at 1.09 for all model executions (to represent the sediment bed). This calculation was based on the sediment porosity of 0.579 and the density of 2.59g/cc, both of which were determined from field sediment samples.

4.2.44 Bed Boundary Condition Time Series Numbers 1-10

Bed boundary condition time series numbers were set to remain at 0 (i.e. steady state).

4.2.45 Groundwater Flow Time Series Numbers 1-10

Groundwater flow time series numbers were all allowed to remain at 0 as all model executions simulated steady state conditions.

4.3 MARS Chemical Fate and Transport Model Results

Chemical fate and transport model simulations were executed for five possible scenarios: uncapped sediment, sediment capped with sand, sediment capped with Aquablok and a sand bioturbation layer, sediment capped with apatite and a sand bioturbation layer, and sediment capped with coke breeze and a sand bioturbation layer. Total flux of phenanthrene to the water column from the sediment bed were projected for typical year flow regimes as low return interval storms did not appear to drastically affect cap stability and performance.

4.3.1 Chemical Fate and Transport Model Results

A review of model projections for cumulative phenanthrene mass to the overlying water column reveals that both the Aquablok and coke breeze capping barriers appear to be highly effective in retarding the migration of phenanthrene from the sediment bed to the water column. The effectiveness of the Aquablok barrier was expected as the material has been developed to control advective contaminant migration and the demonstration area is prone to high advective flow rates. Coke breeze, with its high sorptive capacities for organic compounds, was equally effective in controlling the release of phenanthrene from the sediment bed. Consultations with researchers familiar with the partitioning properties of the coke material have revealed that adjusting the fraction organic carbon input within the model is a reasonable means of representing the sorptive abilities of the coke breeze cap (Lowry, 2004).

Both the apatite and traditional sand caps experienced a contaminant release to the water column at approximately 60 days. Based on the partitioning characteristics of phenanthrene, the depth of the capping layer, and the high advective flow rate (5.5 cm/day), this model projection is accurate when compared to theoretical migration times. The apatite and sand barriers displayed similar effectiveness in retarding the migration of phenanthrene as both materials have relatively similar organic compound partitioning qualities.

Results from model simulations can be seen in Figure 4.1 and calculated phenanthrene flux rates (at the sediment-water interface) for each capping material can be found in Table 4.6. Flux rates were calculated for the period of day 360 through day 1800.

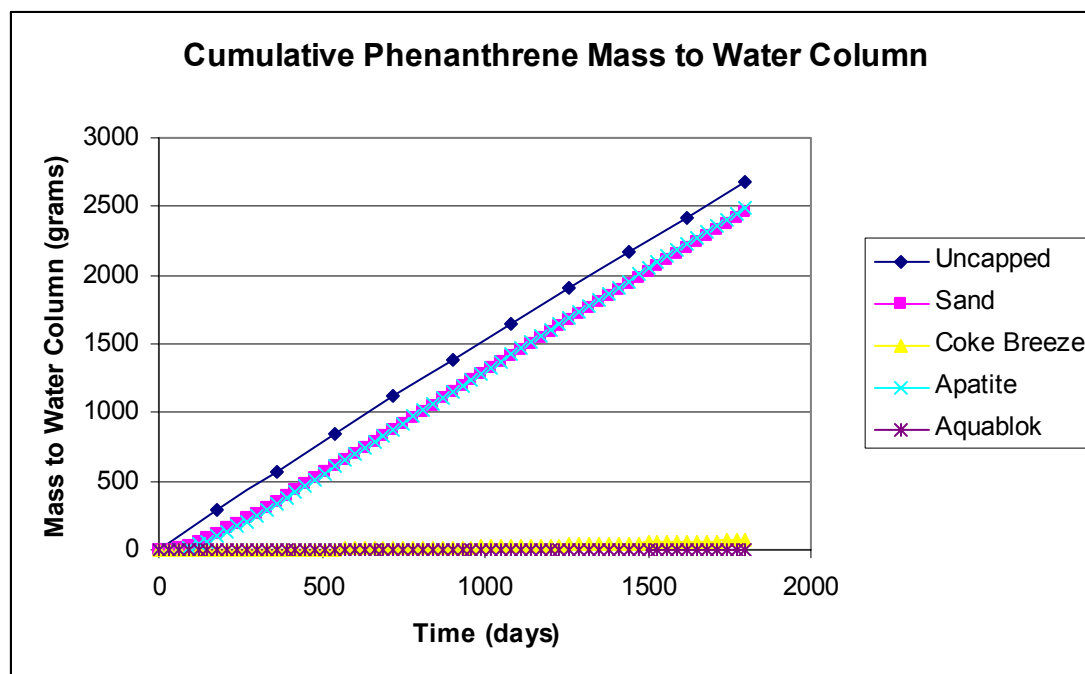


Figure 4.1: Phenanthrene Mass to Water Column

An additional analysis was performed to determine the effective of the groundwater flow rate on the rate of contaminant release to the water column. Model simulations were conducted assuming no cap and uniform 16 mg/kg contaminant concentration through the sediment bed.

Groundwater flow rates were then set to 5.5 cm/day, 2.25 cm/day, and 0 cm/day. The results from these analyses can be seen in Table 4.7.

Table 4.6: Steady-State Phenanthrene Flux Rates at Sediment-Water Interface

Material:	Sand	Coke Breeze	Apatite	Aquablok
Flux Rate (mg/d-m ²)	0.49	0.02	0.50	5.7E-6

Table 4.7: Phenanthrene Flux at Varying Groundwater Rates

Groundwater Flow Rate (cm/day):	0.00	2.25	5.50
Phenanthrene Flux at Sediment-Water Interface (mg/d-m ²)	0.02	0.27	0.53

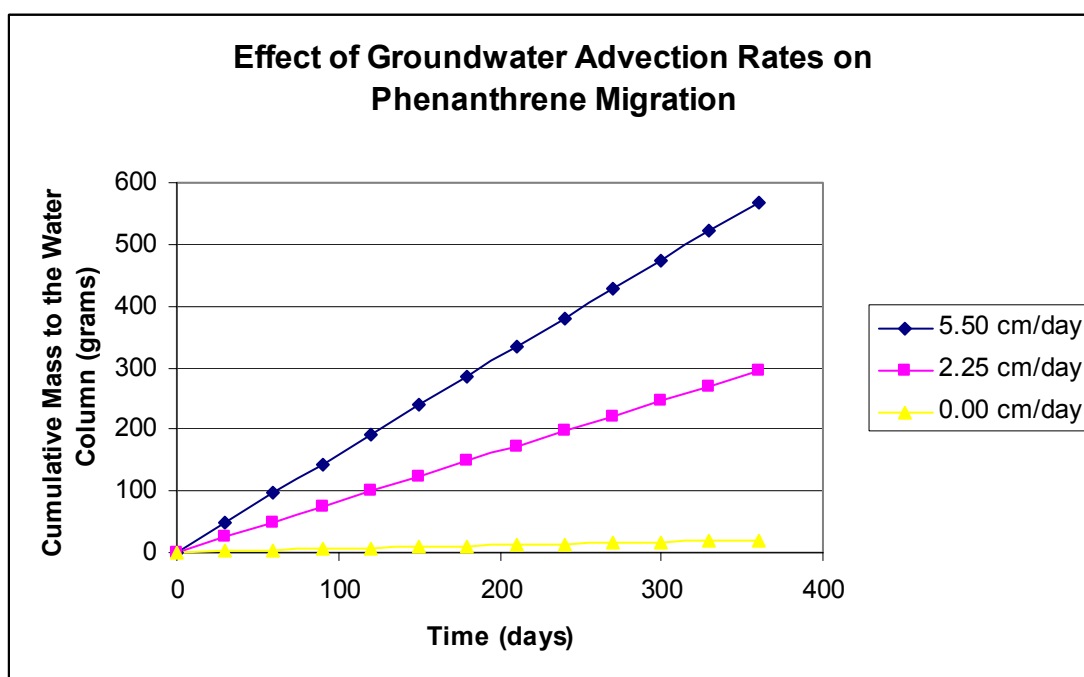


Figure 4.2: Effect of Groundwater Advection on Phenanthrene Release

4.4 Conclusions and Recommendations for Future Improvements

4.4.1 Conclusions

As expected, the sand caps delayed contaminant migration to the water column by approximately 60 days before breakthrough occurred. Due to the relatively high advective flow

rates which were used to constrain the model, it was expected that the sand cap would have only a limited effect on the chemical fate and transport of the contaminants of concern. Under field conditions, it is reasoned that sand caps in the Anacostia will have a greater effect on slowing chemical movement to the water column.

Aquablok performed better than expected as it relates to retardation of chemical migration. Projections illustrate a near zero-flux scenario for all contaminants when capped using the Aquablok product. While this would seem reasonable considering the high advective fluxes present in the Anacostia sediments due to local tidal pumping, it would also appear that Aquablok caps would be prone to severe losses in effectiveness if punctured since this capping technology requires on retardation of groundwater flow and has little sorptive capacity.

Apatite's relative lack of retardation of phenanthrene movement to the water column was expected as the target contaminants for phosphate-based active capping are heavy metals. As MARS currently has no heavy metal modeling capabilities, apatite was not expected to exhibit any favorable capping characteristics for PAHs and PCBs.

The effectiveness of the coke breeze in limiting phenanthrene migration to the water column was expected as coke has shown PCB sorptive qualities in laboratory experiments. Communications with Dr. Greg Lowry of Carnegie Mellon University have indicated that the best means of representing the sorptive abilities of the coke product may be by using a Freundlich Isotherm K_f value of 4.66 and a $1/n$ value of 0.84 (Murphy, 2004). As MARS does not appear to explicitly have the ability to represent this quality, it may be considered for addition to future models. The Freundlich Isotherm model is as follows (Watts, 1997):

$$C_s = \frac{x}{m} = K_f C_e^{1/N} \quad (\text{Equation 4.4-1})$$

Where: C_s = Contaminant concentration sorbed on solid (dimensionless)

x = mass of material sorbed on solid phase (g)
 m = mass of sorbate (g)
 K_F = Freundlich sorption coefficient
 C_E = concentration of contaminant remaining in solution at equilibrium (g/m^3)
 N = empirical coefficient

4.4.2 Recommendations for Future Improvements

Recommendations for future improvements to the MARS model include more detailed capping capabilities to allow for active barrier capping scenarios. While the model exhibits excellent capabilities for simulating sand capping and dredge removal, MARS' active capping capabilities are limited. By allowing a more detailed description (i.e., all the same inputs as the sediment layers) of the capping layer, it is believed that MARS would be able to accurately predict the effectiveness of active capping barrier technologies. For ease of input, it is also recommended that groundwater flow be changed from units of volumetric flow (m^3/day) to some form of seepage velocity as most groundwater flow measurements will be found in linear velocity units.

Chapter 5: Comprehensive Review of MARS Modeling Results and Recommendations

The Model for the Assessment and Remediation of Sediments has proven over the course of this research to be a capable, comprehensive means of modeling the Anacostia River and the associated sediment and chemical transport phenomena. With future revisions, it is hoped that MARS will become an even more valuable weapon in the arsenal of those who seek to remediate our world's contaminated waterways and sediment beds.

5.1 Discussion of Hydrodynamic Model Results

5.1.1 Conclusions

MARS hydrodynamic model projections appear to be relatively accurate predictions of river flow velocities when compared to HEC model projections and field measurements, particularly at normal flow stages. As all sediment transport and chemical fate/transport runs were conducted assuming normal flow conditions, these hydrodynamic model results allowed for accurate baseline conditions for those sediment transport and chemical fate/transport runs of particular interest (i.e., normal flow). Those discrepancies that do exist between model projections and field values could be attributed to the inability to accurately represent the tidal influence on river flow velocities.

5.1.2 Recommendations for Future Improvements

The addition of user input for imposing additional boundary conditions on tidal amplitudes at the upstream river boundary would be a beneficial addition to MARS modeling packages. Such a boundary condition would allow for the modeling of shorter river stretches that are under the influence of tidal fluctuations along the entire stretch. This would allow for MARS to be applied to a larger number of river systems.

5.2 Discussion of Sediment Transport Model Results

5.2.1 Conclusions

A review of MARS sediment transport model reveals that the demonstration area for the AACP is typically a zone of sediment deposition and requires no armoring for resistance to cap erosion by normal flow velocities. Additional model simulations indicate that cap armoring in this area of the Anacostia River may be unnecessary as model projections indicate only a minimal erosion of the sediment bed, which would be confined to the uppermost regions of the bioturbation layer.

5.2.2 Recommendations for Future Improvements

The ability of MARS to model non-cohesive sediment transport would be a helpful addition to future versions of the model. While most contaminant transport is associated with cohesive sediments, it is believed that the ability to project the transport of sands by rivers would only further increase the models capabilities. Additionally, the ability to vary erosional characteristics of sediments on a spatial basis would allow projections to more accurately reflect deposition/erosion processes associated with those areas of the river bottom displaying characteristics varying from those of the majority of the river's sediment bed.

5.3 Discussion of Chemical Fate and Transport Results

5.3.1 Conclusions

MARS chemical fate and transport model simulations indicate a high degree of effectiveness in Aquablok and coke breeze abilities to retard phenanthrene migration into the water column. Both apatite and sand were expected to have limited effectiveness in limiting the movement of phenanthrene from the sediment bed to the overlying water column and model simulations resulted in the same projection.

5.3.2 Recommendations for Future Improvements

Active capping barrier capabilities would be a welcome addition to future MARS model. While MARS is adept at modeling chemical fate and transport and simulating capping and dredging remediation technologies, the ability to input all physical parameters of a capping material pertinent to chemical migration would afford MARS the opportunity to be readily employed in active capping projects.

5.4 Recommendations for Future Model Additions

Future additions to subsequent versions of the MARS model will undoubtedly include physical characteristics of PCBs within the chemical wizard and the ability to model the fate and transport of heavy metals in a sediment bed. Those PCB characteristics which may be of use in a future database are available upon request.

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Appendix A: USGS Anacostia River Peak Flows

USGS 01649500 NORTH EAST BRANCH ANACOSTIA RIVER AT RIVERDALE, MD

Peak Flows

Water Year	Date	Gage Height (feet)	Stream- flow (cfs)		Water Year	Date	Gage Height (feet)	Stream- flow (cfs)
1933	Aug. 23, 1933	15.5	10,500		1970	Jul. 09, 1970	5.76	3,240
1939	Jan. 30, 1939	8.53	1,580		1971	Sep. 11, 1971	6.6	4,340
1940	Apr. 20, 1940	10	2,350		1972	Jun. 22, 1972	9.52	12,000
1941	Jul. 13, 1941	7.07	1,350		1973	Jun. 24, 1973	6.16	3,760
1942	Aug. 09, 1942	11.47	2,980		1974	Mar. 30, 1974	6.34	3,990
1943	Oct. 16, 1942	12.93	3,660		1975	Sep. 26, 1975	10.57	10,800
1944	Nov. 09, 1943	9.84	2,280		1976	Jan. 01, 1976	8.14	5,490
1945	Jul. 18, 1945	12.72	3,680		1977	Oct. 25, 1976	6.99	4,050
1946	Dec. 06, 1945	8.65	1,660		1978	Jan. 26, 1978	8.71	6,410
1947	Jun. 14, 1947	9.02	1,820		1979	Sep. 05, 1979	10.16	9,410
1948	Aug. 12, 1948	8.93	1,780		1980	Oct. 01, 1979	7.09	4,170
1949	Nov. 29, 1948	7.52	1,280		1981	Aug. 31, 1981	7.3	4,410
1950	Sep. 11, 1950	9.63	2,060		1982	Jun. 01, 1982	5.03	2,010
1951	Jun. 13, 1951	9.39	1,980		1983	Jun. 19, 1983	8.45	6,010
1952	Sep. 01, 1952	10.64	2,770		1984	Mar. 29, 1984	7.21	4,310
1953	Nov. 22, 1952	11.11	3,000		1985	Sep. 27, 1985	8.04	5,360
1954	Dec. 14, 1953	6.1	889		1986	Aug. 08, 1986	6.19	3,150
1955	Jan. 14, 1955	7.25	3,120		1987	Dec. 24, 1986	8.01	5,320
1956	Oct. 14, 1955	6.38	2,870		1988	May 23, 1988	6.15	3,110
1957	Apr. 05, 1957	4.3	1,020		1989	May 6, 1989	9.56	8,100
1958	Jul. 23, 1958	6.1	3,400		1990	Aug. 06, 1990	6.61	3,610
1959	Aug. 08, 1959	5.49	2,470		1991	Mar. 23, 1991	7.27	4,380
1960	Sep. 12, 1960	5.75	2,830		1992	Jul. 25, 1992	8.03	5,350
1961	Apr. 13, 1961	5.44	2,340		1993	Nov. 23, 1992	6.11	3,060
1962	Mar. 12, 1962	5.15	1,940		1994	Nov. 28, 1993	9.45	7,880
1963	Aug. 20, 1963	6.98	5,060		1995	Jan. 20, 1995	6.9	3,940
1964	Jan. 09, 1964	4.94	1,670		1996	Jan. 19, 1996	9.28	7,540
1965	Mar. 05, 1965	5.42	2,310		1997	Nov. 08, 1996	9.05	7,090
1966	Sep. 14, 1966	7.6	3,300		1998	Mar. 09, 1998	8.93	6,870
1967	Aug. 25, 1967	6.44	4,570		1999	Sep. 16, 1999	9.23	7,440
1968	Sep. 10, 1968	4.61	2,510		2000	Aug. 27, 2000	5.82	2,760
1969	Aug. 10, 1969	7.28	5,660		2002	Sep. 01, 2002	6.49	3,470
					2003	Sep. 23, 2003		5,600

USGS 01651000 NW BRANCH ANACOSTIA RIVER NEAR HYATTSVILLE, MD

Peak Flows

Water Year	Date	Gage Height (feet)	Stream-flow (cfs)		Water Year	Date	Gage Height (feet)	Stream-flow (cfs)
1933	Aug. 24, 1933	13.5			1971	Aug. 27, 1971	9.12	2,510 ^D
1939	Apr. 26, 1939	6.03	1,880		1972	Jun. 22, 1972	14.47	18,000
1940	Apr. 20, 1940	6.48	1,750		1973	Aug. 20, 1973	6.63	3,200
1941	Jul. 13, 1941	5.11	1,050		1974	Mar. 30, 1974	6.22	2,640
1942	Aug. 09, 1942	9.52	2,180		1975	Sep. 26, 1975	11.17	14,800
1943	Oct. 16, 1942	9.92	2,280		1976	Sep. 16, 1976	6.59	5,540
1944	Nov. 09, 1943	8.82	2,000		1977	Oct. 25, 1976	5.36	3,620
1945	Jul. 27, 1945	10.02	2,300		1978	Jan. 26, 1978	5.91	4,440
1946	Jun. 29, 1946	6.41	1,300		1979	Sep. 06, 1979	9.4	12,000
1947	Sep. 06, 1947	6.37	1,300		1980	Oct. 01, 1979	5.27	3,780
1948	Aug. 03, 1948	8.37	1,900		1981	Jun. 14, 1981	4	2,060
1949	May 23, 1949	7.48	1,650		1982	May 28, 1982	4.34	2,470
1950	Sep. 10, 1950	9.86	2,280		1983	Apr. 15, 1983	4.14	2,230
1951	Jun. 13, 1951	9.03	2,130		1984	Mar. 29, 1984	3.89	1,930
1952	Sep. 01, 1952	11.4	3,360		1985	Jul. 12, 1985	5.57	3,520
1953	Nov. 22, 1952	10.16	2,710		1986	Aug. 08, 1986	7.39	7,390
1954	Jun. 15, 1954	10.69	2,980		1987	Dec. 24, 1986	5.86	4,030
1955	Aug. 22, 1955	11.19	2,930		1988	Aug. 06, 1988	4.7	2,190
1956	Oct. 14, 1955	11.32	3,010		1989	May 5, 1989	7.08	6,620
1957	Jun. 05, 1957	9.16	1,550		1990	Aug. 05, 1990	5.6	3,570
1958	Jul. 22, 1958	11.67	3,590		1991	Jul. 25, 1991	6.31	4,900
1959	Aug. 08, 1959	12.12	4,170		1992	Jul. 21, 1992	6.35	4,980
1960	Aug. 04, 1960	11.31	3,180		1993	Nov. 23, 1992	4.5	1,930
1961	Apr. 13, 1961	9.68	2,210		1994	Nov. 28, 1993	7.79	8,340
1962	May 31, 1962	8.82	1,810		1995	Jul. 07, 1995	5.63	4,340
1963	Aug. 20, 1963	11	3,200		1996	Sep. 06, 1996	6.94	6,650
1964	Nov. 06, 1963	8.6	1,700		1997	May 25, 1997	6.31	5,500
1965	Mar. 05, 1965	9.82	2,390		1998	Mar. 09, 1998	4.44	2,560
1966	Sep. 14, 1966	13.5	7,000		1999	Sep. 16, 1999	5.77	4,570
1967	Aug. 25, 1967	12.67	5,030		2000	Aug. 27, 2000	4.1	2,150
1968	Jan. 14, 1968	8.38	1,900		2001	Aug. 23, 2001	4.77	3,010
1969	Aug. 10, 1969	13.2	6,050		2002	Sep. 01, 2002	3.68	1,710
1970	Jul. 09, 1970	10.53	3,220		2003	Sep. 23, 2003	7.24	7,230

Appendix B: Geochronological Analyses

Results of Geochronological Analyses of Anacostia River Multicores

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Introduction

Objective

This report summarizes results of X-radiographic and ^{210}Pb , ^{137}Cs and ^7Be geochronological analyses of multicores collected from the lower Anacostia River in March 2003. The purpose of this study is to constrain the sediment-accumulation and the sediment-bioturbation rates in the upper 0-40cm and 0-5cm of the cores, respectively.

Analytical Methods

Multicores were collected from the study area and subsampled for X-radiography and radioisotopes. Samples for X-radiography were obtained by pushing open-ended, three-sided Plexiglas trays (2.0 cm thick) into core boxes on deck, then inserting the fourth side, so as to minimize fabric distortion (Kuehl et al., 1988). Slabs were sealed with neoprene plugs and electrical tape and transported to the laboratory for imaging. Slabs were imaged using a Medison Acoma PX15-HF X-ray generator (1.2 second exposures at 60KeV, 12mA), and a Thales Flashscan 35 Digital X-ray Detector panel for image capture, with 14-bit dynamic resolution and 127 micron pixel size.

Sedimentation analyses on accumulation rates were estimated using ^{210}Pb , and ^{137}Cs while biodiffusion rates were estimated using ^7Be geochronology. Multicore subcores were extruded in the field at depth intervals of 1 or 2 cm, dried at 70°C , and then sealed in airtight plastic container for three weeks prior to analysis. These procedures allow the ingrowth of radionuclides ^{222}Rn , ^{214}Pb , and ^{214}Bi , which are the parent isotopes of ^{210}Pb in the ^{238}U decay chain. The ingrowth radionuclides parent isotopes are necessary in turn to discriminate the activity of the supported ^{210}Pb , which produced by ^{226}Ra - ^{222}Rn decay in the crystal lattices of sediment particles, from excess ^{210}Pb , which supplied from the water column.

Activities of ^{210}Pb (natural product of U-series decay with $t_{1/2} = 22.3$ years), ^{137}Cs (product of nuclear fission in nuclear reactors and bombs with $t_{1/2} = 30.7$ years) and ^7Be (product of cosmic-ray spallation of nitrogen and oxygen in the earth's atmosphere with $t_{1/2} = 53.3$ days) were determined by γ -spectroscopy analysis on dried sediment with the photopeaks indicated at 46.5 KeV for ^{210}Pb , 661 KeV for ^{137}Cs and 477.7 KeV for ^7Be . Three LEGe detectors (Canberra Instruments model GL2020R and GL3825R) were used.

^{210}Pb activities were corrected for self-adsorption by calibration with standards of known activity (Cutshall et.al., 1983). Excess activities of ^{210}Pb were determined by comparison with supported activities of parent radionuclides ^{214}Pb , with photopeaks at 295 and 351 KeV and ^{214}Bi , with a primary photopeak at 609 KeV. The minimum detection limits for ^{137}Cs was 0.04dpm/g in 20-g samples. Activities of ^7Be were calibrated using a linear efficiency calibration curve derived from NIST SRM standards containing ^{214}Pb , ^{214}Bi , and ^{137}Cs (over the energy range 295-661 KeV).

Accumulation rates (S, cm/yr) and biodiffusion coefficients (Db, cm^2/yr) were calculated from ^{210}Pb and ^7Be gradients, respectively, using least squares fits to end-member solutions of advection-diffusion-reaction equation (Aller and Cochran, 1976; Nittrouer and Sternberg, 1981). Minimum accumulation rates were also calculated based on penetration depth of ^{137}Cs into the riverbed.

In the ^{210}Pb model, if the accumulation process is assumed to be the dominant process with steady state conditions (e.g., Nittrouer et al., 1984), where there were no sediment mixing (physical or biological) occurred in the core, the accumulation rate, S can be determined as:

$$A(z) = A(0) e^{\left(\frac{-z \cdot \lambda}{S} \right)} \quad [1]$$

Since the physical mixing and biodiffusion rate were assumed to be negligible, the resulting accumulation rates determined from Eq. [1] should be considered maximum value.

Subsequently, if the biodiffusion process is assumed to be the dominant process over the time- and length- scales of interest, with steady state condition, where the accumulation process can be ignored in the core, the biodiffusion coefficient, D_b can be determined as:

$$A(z) = A(0) e^{\left(\frac{-z}{\sqrt{\frac{D_b}{\lambda}}} \right)} \quad [2]$$

Where,

λ = decay constant for the radionuclide of interest, 1/yr

A= excess activity, dpm/g

z= depth of the sediment, cm

S= accumulation rate, cm/yr

D_b =biodiffusion coefficient, cm^2/yr

Since all the transport of ^7Be was assumed to be a result of steady state biodiffusive mixing of sediment particles only, the resulting biodiffusion coefficient determined from Eq. [2] should also be considered maximum value. If physical mixing or accumulation were significant, the actual value of D_b would be lower.

In the ^{137}Cs model, ^{137}Cs was assumed to be first introduced into environment in 1954, and was transport to depositing sediments, and reached the peak activities in the atmosphere in 1963. In addition, the biodiffusion process was also assumed to be negligible, and hence no depth correction for ^{137}Cs data was required. Thus, the accumulation rate, S, from ^{137}Cs model can be determined by subtracting the depth of rapid biodiffusion estimated from ^7Be profile (~5cm for all stations) from the total penetration depth, and dividing by the elapsed time between the first releases of ^{137}Cs reaches into the atmosphere (year 1953) and the date of core collection as shown below:

$$S \text{ (cm/yr)} = \frac{[(\text{depth of max. } ^{137}\text{Cs}) - \text{depth of biodiffusion, cm}]}{(2003-1953, \text{ yr})} \quad [3]$$

Because ^{137}Cs penetrated to be bottom of all cores analyzed, the rates given in Figure 1 are minimum estimates only.

Results and Discussion

X-radiography. X-radiographic images of cores are shown in Figure 2. Images are negatives, wherein high density sediments (sand and gravel) are light shades of gray, and lower density particles (mud and organics) are shown in darker shades. Cracks are clearly visible, and were produced primarily by leaves and plastic debris that disturbed core fabric as Plexiglas trays were inserted into subcores. Some additional cracking may have occurred while samples were being transported from the field to the lab. Overall sedimentary fabric for all four cores is characterized by faint mottling (probably produced by bioturbation) overprinting stratification (produced during sediment deposition and physical mixing/sedimentation). Qualitatively, such fabric indicates that sediment mixing rates from bioturbation are comparable to or slightly more intense than the combined effects of sediment deposition and physical reworking. Also, because each region of physical stratification appears to have been overprinted by biogenic activity, it is likely that bioturbation reworks sediment to greater depths than do physical processes alone (e.g., Bentley and Nittrouer, 2003; Bentley and Sheremet, 2003).

Radioisotopes. Radiochemical analyses were conducted for cores A2-2, A3-2 and A4-2 as summarized in Table 1. Sediments in cores A1-2, A6-1 and A6-2 (refer Table 2 for location details), were too coarse to merit radiochemical analysis.

	Latitude				Longitude			Maryland State Plane Coordinates NAD83	
Station ID, No. Cores, Time (EST)	Deg.	Min.	Sec.		Deg.	Min.	Sec.	Easting(ft)	Northing(ft)
A2-2 cores@1105	38	52	18.7555		77	0	15.5574	1311103.0	438921.0
A3-2 cores@1200	38	52	17.4527		77	0	17.3454	1310961.6	438789.2
A4-2 cores@1445	38	52	17.4499		77	0	14.1729	1311212.5	438788.9

Table 1: Location of the cores with sampling analysis.

	Latitude				Longitude			Maryland State Plane Coordinates NAD83	
Station ID, No. Cores, Time (EST)	Deg.	Min.	Sec.		Deg.	Min.	Sec.	Easting(ft)	Northing(ft)
A1-2 cores@1010	38	52	19.7085		77	0	13.029 6	1311302.9	439017.4
A6-1 core@1345	38	52	18.0083		77	0	15.301 3	1311123.2	438845.4
A6-2 cores@1517	38	52	18.5116		77	0	15.501 4	1311107.4	438896.3

Table 2: Location of the cores without sampling analysis.

Station	²¹⁰ Pb Accumulation rate, S (cm/yr)	Correlation Coefficient, r^2	¹³⁷ Cs Accumulation rate, S (cm/yr)	Biodiffusion Coefficient, D _b (cm ² /yr)	Correlation Coefficient, r^2
A2-2	0.66	0.84	>0.4	24	0.86
A3-2	1.00	0.48	>0.8	34	0.88
A4-2	0.61	0.79	>0.7	29	0.67

Table 3: Summary of the accumulation rates and biodiffusion coefficient.

Biodiffusion coefficients, D_b were calculated for all the cores using Eq. [2]. We assumed that rapid mixing (i.e., sediment mixing over seasonal timescales, 3-5 half-lives of ⁷Be) was restricted to the depth range containing detectable ⁷Be, and that the mixing is mainly particle alone without pore fluid. As a result, biodiffusion coefficients were not corrected for porosity gradients near the sediment-water interface (e.g., Boudreau, 1997). Such corrections were impeded by apparently high and variable organic content in all cores, resulting from twigs, leaves, and other carbonaceous debris found in cores. The calculated biodiffusion coefficients, D_b ranges from 24 cm²/yr to 34 cm²/yr with the correlation coefficient, r^2 ranges from 0.67 to 0.88 (Table 3). The range of calculated biodiffusion coefficients is relatively small, suggest lateral uniformity in mixing intensity over the spatial scale of 10-100 m.

Accumulation rates for all cores were estimated based on least-squares fit of Eq. [1] (²¹⁰Pb estimation) to the region of exponential activity decline below ~5 cm (Fig 1). The profile of A2-2 and A4-2 yield an accumulation rate of 0.66 cm/yr and 0.61 cm/yr with a correlation coefficient, r^2 of 0.84 and 0.79, respectively. The accumulation rate of A3-2 was 1.00 cm/yr with correlation coefficient, r^2 of 0.48. Complete ¹³⁷Cs profiles for cores of A2-2 and A4-2 were also shown in Figure 1. Minimum accumulation rates estimated by ¹³⁷Cs (Eq. 3) for A2-2, A3-3 and A4-2 were >0.44, >0.84, and >0.76 cm/yr, and generally corroborate estimates of accumulation rate from the ²¹⁰Pb method.

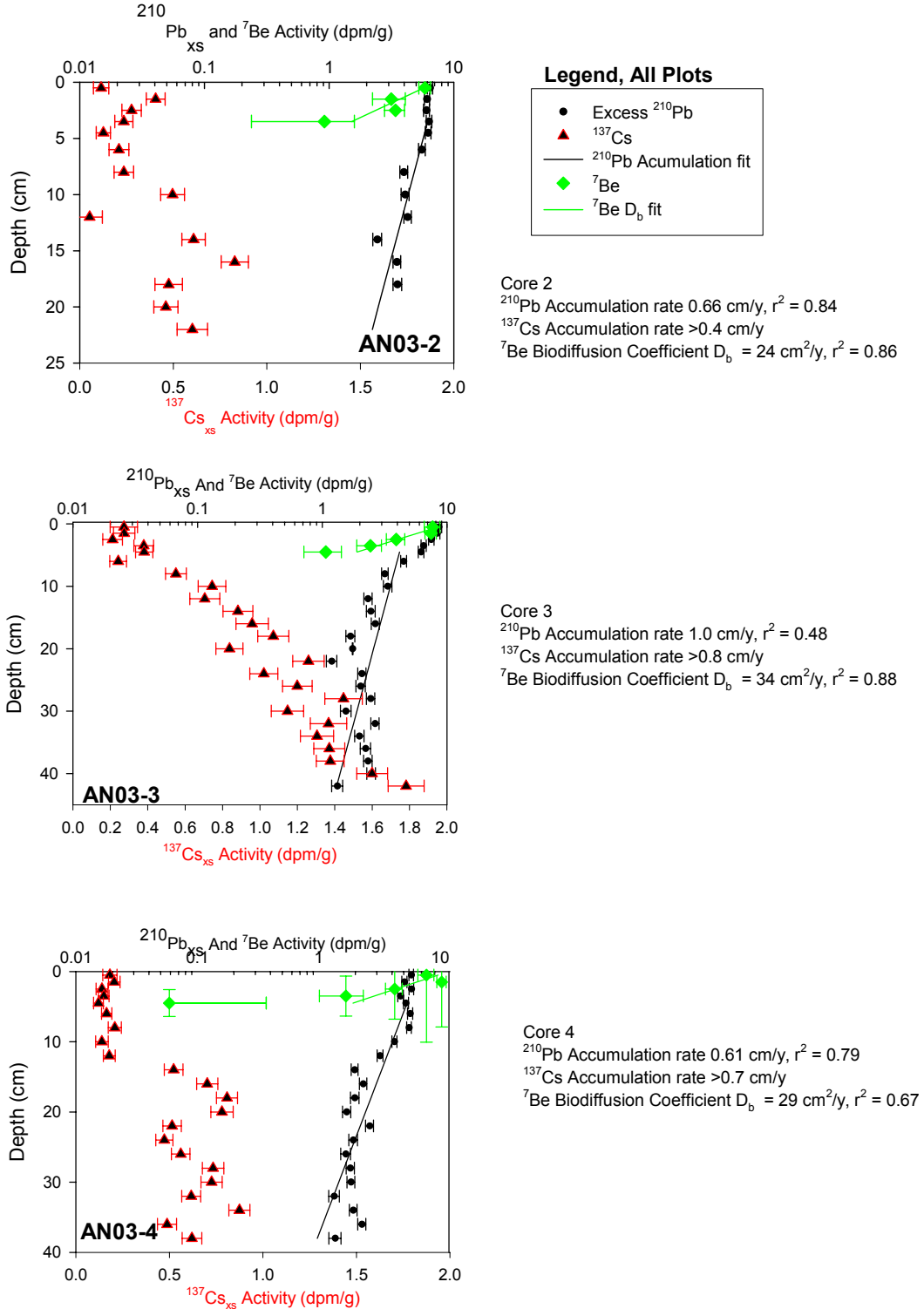


Figure 1: ^{210}Pb , ^{137}Cs , and ^7Be profiles and model fits for equations 1 and 2. For ^{137}Cs accumulation rates, bioturbation depths were estimated at 4-5 cm, from ^7Be data.

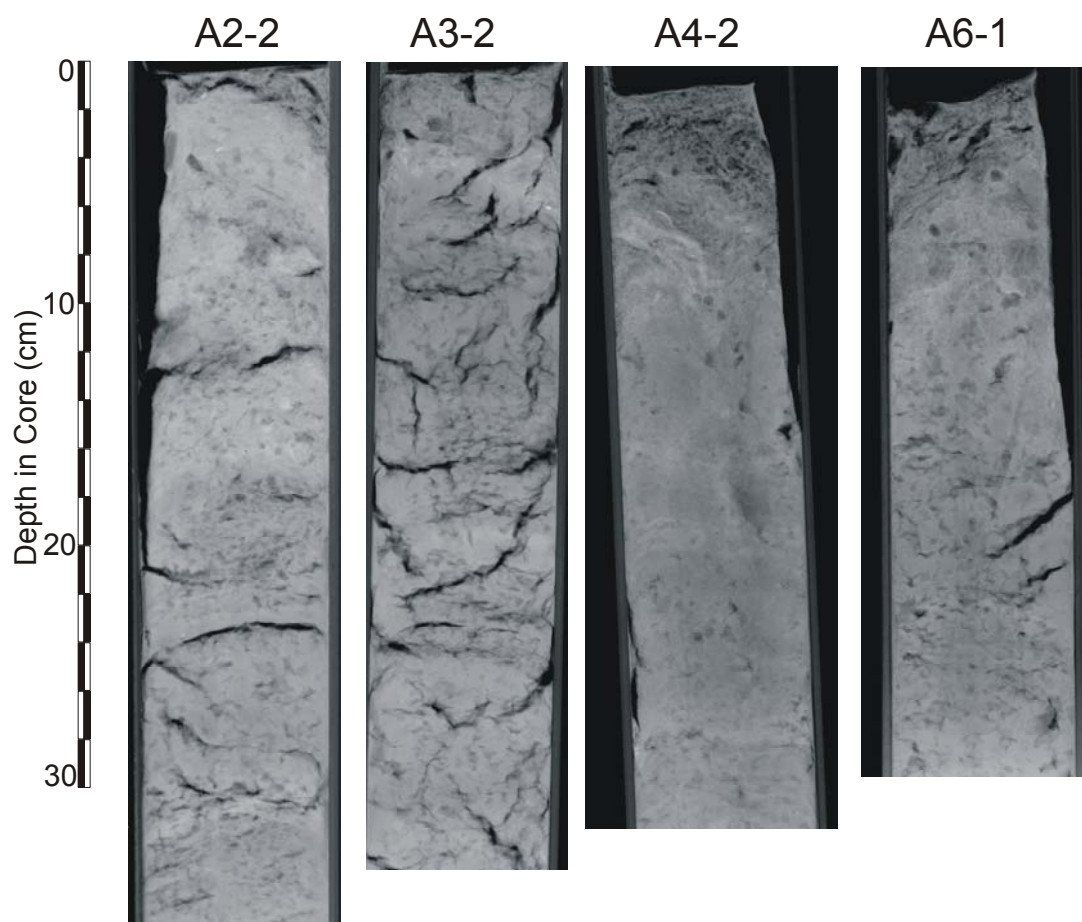


Figure 2. X-radiographic images of cores from the lower Anacostia River. The riverbed/sediment-water interface is indicated by 0-cm depth on the scale bar.

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Appendix C: Coring Contaminant Concentrations

Depth below Sediment-water interface (in)	Chemical Concentrations (ug/kg)		
	Benzo (a) pyrene	Phenanthrene	Pyrene
0-6	4700	16000	13000
	4600	15000	12000
	4400	8000	9900
	3900	6000	8300
	3800	5100	7800
	3800	5000	6700
	3700	5000	6600
	3600	4500	6300
	3500	4400	6300
	3400	4400	6200
	3200	4300	6200
	3200	4200	5800
	3100	4200	5700
	3100	4100	5500
	3000	3900	5500
	3000	3900	5400
	2900	3900	5000
	2900	3900	5000
	2900	3900	4900
	2700	3800	4900
	2700	3700	4800
	2700	3700	4800
	2600	3700	4800
	2500	3600	4800
	2500	3500	4700
	2500	3400	4600
	2500	3300	4500
	2500	3100	4500
	2400	3100	4300
	2400	3000	4300
	2400	2900	4200
	2400	2900	4200
	2300	2800	4000
	2300	2800	4000
	2300	2800	3900
	2300	2700	3900
	2200	2700	3900
	2100	2700	3700
	2100	2600	3600
	2100	2500	3600
	2100	2500	3500
	2100	2500	3500
	2000	2500	3400
	2000	2400	3400

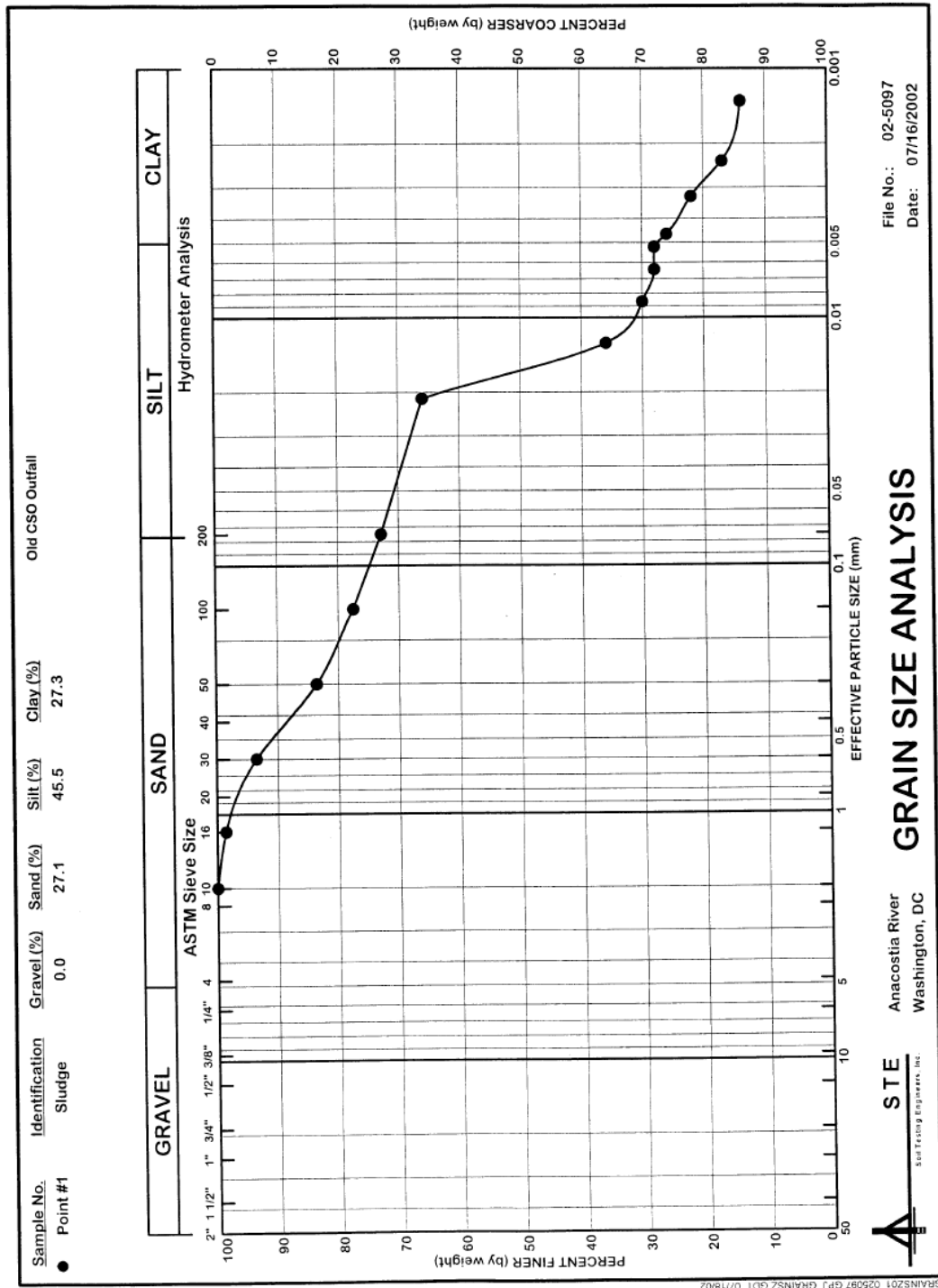
	2000	2400	3300
	2000	2300	3300
	1900	2200	3300
	1800	2200	3200
	1800	2200	3000
	1800	2100	2900
	1800	2100	2800
	1800	2100	2800
	1800	2100	2800
	1700	2100	2700
	1700	1900	2500
	1700	1800	2300
	1600	1800	2200
	1400	1700	2100
	1400	1700	2100
	1400	1700	2100
	1300	1500	2000
	1200	1500	2000
	1200	1400	1900
	1100	1400	1800
	1100	1300	1800
	1100	1200	1800
	1100	1100	1500
	1100	1100	1500
	1000	1000	1500
	950	1000	1200
	740	950	1200
	710	940	1100
	580	920	890
	560	660	830
	440	660	180
6-12	3000	6800	5400
	1600	2300	2700
	1600	2000	2700
	1100	1700	1800
	780	1300	1500
	710	1300	1400
	550	980	1000
	360	710	810
12-deep	3700	5400	6600
	1900	4000	4800
	1500	2300	2700
	1200	1800	2100
	1200	1200	2100
	710	930	1300
	410	620	780

	Chemical Concentrations (ug/kg)		
Depth below Sediment- water interface (in)	Bz# 8	Bz# 31	Bz# 70
0-6	100	290	150
	62	200	110
	58	200	110
	43	150	110
	34	120	84
	30	100	82
	20	95	60
	19	82	50
6-12	92	310	180
	47	180	120
	44	170	110
	40	150	100
	14	74	75
		59	62
		53	51
		40	
12-deep	58	260	160
	37	150	100
	27	130	100
	2.1	20	18
		12	4.9
		6.8	
		6.5	

Appendix D: Sediment Geotechnical Analysis

Initial analysis of the physical composition of grab sediment samples from the demonstration area revealed a percentage make-up (by weight) of 27.1% sand (approximately 5mm - 0.075mm effective particle size), 45.5% silt (approximately 0.075mm - 0.005mm effective particle size), and 27.3% clay (approximately 0.005 mm and smaller effective particle size). The d_{50} for the grab sample was 0.018 mm effective particle size and can be seen in Figure A-1 (Soil Testing Engineers, 2002). Based on these analyses, the demonstration area appears to be overlain by fairly fine, cohesive sediment. The sediment make-up appears to be consistent with little spatial variation in surface sediment texture (Earth Resources Technology, Inc., 2003).

Figure A-1: Anacostia Sediment Geotechnical Characterization



Source: Soil Testing Engineers, 2002

Vita

Keegan L. Roberts was born on January 22, 1979, in Metairie, Louisiana. He graduated from his high school, Archbishop Hannan High School, in May 1997. Following high school he attended Louisiana State University where he earned a Bachelor of Science degree in Civil Engineering in December 2001. Keegan has been a fulltime graduate student at Louisiana State University in the Department of Civil and Environmental Engineering since December 2001 and is presently a candidate for the degree of Master of Science in Civil Engineering.